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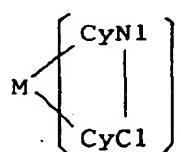
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(54) Metal coordination compound, luminescence device and display apparatus

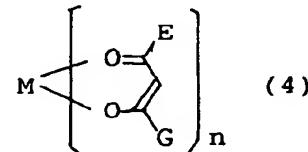
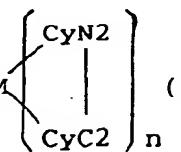
(57) An electroluminescence device having a layer containing a specific metal coordination compound is provided. The metal coordination compound is represented by formula (1) below:



wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure ML_m is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3) or (4) shown below:

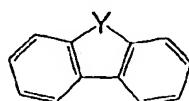


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at least one of the optional substituent(s) of the cyclic groups, and the cyclic groups CyC1 and CyC2 include an aromatic group capable of having a substituent represented by the following formula (5):



EP 1 238 981 A2

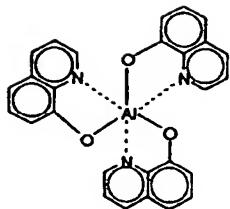
The metal coordination compound having the aromatic group is effective in providing high-efficiency luminescence and long-term high luminance.

DescriptionFIELD OF THE INVENTION AND RELATED ART

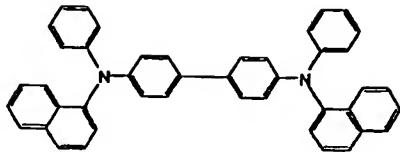
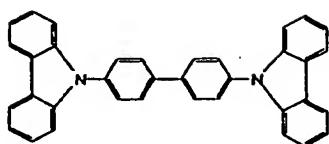
- 5 [0001] The present invention relates to an organic luminescence device (also called an organic electroluminescence device or organic EL device) for use in a planar light source, a planar display, etc. Particularly, the present invention relates to a novel metal coordination compound and a luminescence device having a high luminescence efficiency and causing little change with time by using a metal coordination compound represented by formula (1) appearing hereinafter.
- 10 [0002] An old example of organic luminescence device is, e.g., one using luminescence of a vacuum-deposited anthracene film (Thin Solid Films, 94 (1982) 171). In recent years, however, in view of advantages, such as easiness of providing a large-area device compared with an inorganic luminescence device, and possibility of realizing desired luminescence colors by development of various new materials and drivability at low voltages, an extensive study thereon for device formation as a luminescence device of a high-speed responsiveness and a high efficiency, has been conducted.
- 15 [0003] As precisely described in Macromol. Symp. 125, 1 - 48 (1997), for example, an organic EL device generally has an organization comprising a pair of upper and lower electrodes formed on a transparent substrate, and organic material layers including a luminescence layer disposed between the electrodes.
- 20 [0004] In the luminescence layer, aluminum quinolinol complexes (inclusive of Alq3 shown hereinafter as a representative example) having an electron-transporting characteristic and a luminescence characteristic, are used for example. In a hole-transporting layer, a material having an electron-donative property, such as a triphenylamine derivative (inclusive of α -NPD shown hereinafter as a representative example), is used for example.
- 25 [0005] Such a device shows a current-rectifying characteristic such that when an electric field is applied between the electrodes, holes are injected from the anode and electrons are injected from the cathode.
- [0006] The injected holes and electrons are recombined in the luminescence layer to form excitons, which emit luminescence when they are transitioned to the ground state.
- 30 [0007] In this process, the excited states include a singlet state and a triplet state and a transition from the former to the ground state is called fluorescence and a transition from the latter is called phosphorescence. Materials in these states are called singlet excitons and triplet excitons, respectively.
- [0008] In most of the organic luminescence devices studied heretofore, fluorescence caused by the transition of a singlet exciton to the ground state, has been utilized. On the other hand, in recent years, devices utilizing phosphorescence via triplet excitons have been studied.
- [0009] Representative published literature may include:
- 35 Article 1: Improved energy transfer in electrophosphorescent device (D.F. O'Brien, et al., Applied Physics Letters, Vol. 74, No. 3, p. 422 (1999)); and
Article 2: Very high-efficiency green organic light-emitting devices based on electrophosphorescence (M.A. Baldo, et al., Applied Physics Letters, Vol. 75, No. 1, p. 4 (1999)).
- 40 [0010] In these articles, a structure including four organic layers sandwiched between the electrodes, and the materials used therein include carrier-transporting materials and phosphorescent materials, of which the names and structures are shown below together with their abbreviations.
- 45 Alq3: aluminum quinolinol complex
 α -NPD: N4,N4'-di-naphthalene-1-yl-N4,N4'-diphenyl-biphenyl-4,4'-diamine
CBP: 4,4'-N,N'-dicarbazole-biphenyl
BCP: 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline
PtOEP: platinum-octaethylporphyrin complex
Ir(ppy)₃: iridium-phenylpyrimidine complex

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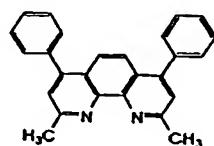
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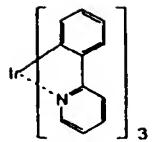
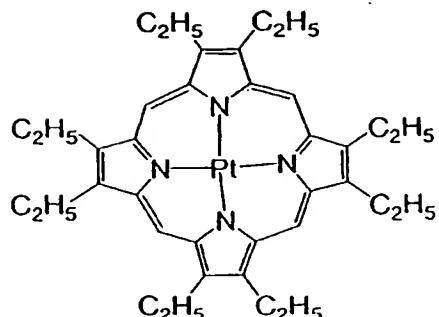
Alq3

 α -NPD

CBP



BCP

Ir(ppy)₃

PtOEP

45 [0011] The above-mentioned Articles 1 and 2 both have reported structures, as exhibiting a high efficiency, including a hole-transporting layer comprising α -NPD, an electron-transporting layer comprising Alq3, an exciton diffusion-preventing layer comprising BCP, and a luminescence layer comprising CBP as a host and ca. 6 % of PtOEP or Ir(ppy)₃ as a phosphorescent material dispersed in mixture therein.

50 [0012] Such a phosphorescent material is particularly noted at present because it is expected to provide a high luminescence efficiency in principle for the following reasons. More specifically, excitons formed by carrier recombination comprise singlet excitons and triplet excitons in a probability ratio of 1:3. Conventional organic EL devices have utilized fluorescence of which the luminescence efficiency is limited to at most 25 %. On the other hand, if phosphorescence generated from triplet excitons is utilized, an efficiency of at least three times is expected, and even an efficiency of 100 %, i.e., four times, can be expected in principle, if a transition owing to intersystem crossing from a singlet state having a higher energy to a triplet state is taken into account.

55 [0013] However, like a fluorescent-type device, such an organic luminescence device utilizing phosphorescence is generally required to be further improved regarding the deterioration of luminescence efficiency and device stability.

[0014] The reason of the deterioration has not been fully clarified, but the present inventors consider as follows based

on the mechanism of phosphorescence.

[0015] In the case where the luminescence layer comprises a host material having a carrier-transporting function and a phosphorescent guest material, a process of phosphorescence via triplet excitons may include unit processes as follows:

- 5 1. transportation of electrons and holes within a luminescence layer,
2. formation of host excitons,
3. excitation energy transfer between host molecules,
4. excitation energy transfer from the host to the guest,
- 10 5. formation of guest triplet excitons, and
6. transition of the guest triplet excitons to the ground state and phosphorescence.

[0016] Desirable energy transfer in each unit process and luminescence are caused in competition with various energy deactivation processes.

15 [0017] Needless to say, a luminescence efficiency of an organic luminescence device is increased by increasing the luminescence quantum yield of a luminescence center material.

[0018] Particularly, in a phosphorescent material, this may be attributable to a life of the triplet excitons which is longer by three or more digits than the life of a singlet exciton. More specifically, because it is held in a high-energy excited state for a longer period, it is liable to react with surrounding materials and cause polymer formation among the excitons, thus incurring a higher probability of deactivation process resulting in a material change or life deterioration.

20 [0019] A luminescence device is desired to exhibit high efficiency luminescence and show a high stability. Particularly, it is strongly desired to provide a luminescence material compound which is less liable to cause energy deactivation in a long life of excited energy state and is also chemically stable, thus providing a longer device life.

25 SUMMARY OF THE INVENTION

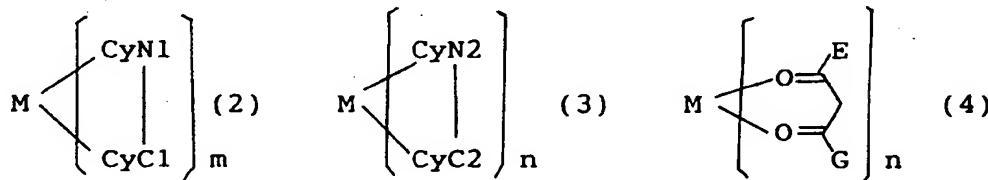
[0020] Accordingly, principal objects of the present invention are to provide a luminescence material which exhibits a high luminescence efficiency and retains a high luminance for a long period, and also provide a luminescence device and a display apparatus using the same.

30 [0021] In the present invention, a metal complex is used as a luminescence material, particularly a novel luminescent metal complex compound comprising iridium as a center metal and an aromatic group of formula (5) appearing hereinafter as a part of a ligand or as a substituent of a ligand.

[0022] More specifically, the present invention provides as a luminescence material a metal coordination compound 35 represented by formula (1) below:



40 wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure ML_m is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3) or (4) shown below:



45 wherein CyN1 and CyN2 are each cyclic group capable of having a substituent, including a nitrogen atom and bonded to the metal atom M via the nitrogen atom; CyC1 and CyC2 are each cyclic group capable of having a substituent, including a carbon atom and bonded to the metal atom M via the carbon atom with the proviso that the cyclic group CyN1 and the cyclic group CyC1 are bonded to each other via a covalent bond and the cyclic group CyN2 and the cyclic group CyC2 are bonded to each other via a covalent bond;

the optional substituent of the cyclic groups is selected from a halogen atom, cyano group, a nitro group, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom);

E and G are independently a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 - 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom; and

at least one of the optional substituent(s) of the cyclic groups, and the cyclic groups CyC1 and CyC2 include an aromatic group capable of having a substituent represented by the following formula (5):

20



25

wherein the aromatic group of the formula (5) is bonded to CyN1, CyN2, CyC1 or CyC2 via a single bond when the aromatic group is the optional substituent(s) of the cyclic groups, and the aromatic group of the formula (5) is bonded to CyN1 or CyN2 via a single bond and bonded to the metal atom M via a single bond when the aromatic group is CyC1 or CyC2;

Y denotes C=O, CRR', C=C(CN)₂, O or S wherein R and R' are independently a hydrogen atom, a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 - 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom); and

the optional substituent of the aromatic group of the formula (5) is selected from a halogen atom, cyano group, a nitro group, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom) with the proviso that an adjacent pair of substituents can be bonded to form a cyclic structure.

[0023] Preferred embodiments of the metal coordination compound of the formula (1) according to the present invention include the following:

- 55 A metal coordination compound having a partial structure ML'_n represented by the formula (3) in the formula (1).
- A metal coordination compound having a partial structure ML'_n represented by the formula (4) in the formula (1).
- A metal coordination compound, wherein n is 0 in the formula (1).
- A metal coordination compound, wherein the group Y in the formula (5) is C=O or CRR'.
- A metal coordination compound wherein the cyclic groups CyC1 in the formula (1) and CyC2 in the formula (3)

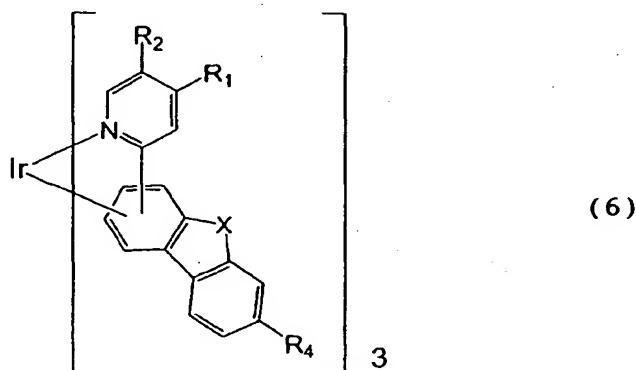
are independently selected from phenyl group, thienyl group, thianaphthyl group, naphthyl group, pyrenyl group, 9-fluorenonyl group, fluorenyl group, dibenzofuryl group, dibenzothienyl group, or carbazolyl group, as an aromatic cyclic group capable of having a substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom, particularly selected from phenyl group or 2-fluorenyl group.

5 A metal coordination compound, wherein the cyclic groups CyN1 in the formula (2) and CyN2 in the formula (3) are independently selected from pyridyl group, pyridazinyl group, and pyrimidinyl group, particularly pyridyl group, as an aromatic cyclic group capable of having a substituent.

10 A metal coordination compound, wherein the cyclic groups CyN1, CyN2, CyC1 and CyC2 are independently non-substituted, or have a substituent selected from a halogen atom and a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom or a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom)), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom).

15 [0024] A metal coordination compound, wherein M in the formula (1) is iridium.

[0025] A metal coordination compound represented by the following formula (6):



35 wherein X denotes CRR', O or S where R and R' are independently a linear or branched alkyl group of formula: C_nH_{2n+1} - in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom;

40 [0026] R2 denotes a hydrogen atom; a fluorine atom; a linear or branched alkyl group of formula: C_nH_{2n+1} - in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom; a phenyl group capable of having a substituent; a 9,9-dialkylfluorenyl group (of which the alkyl groups are independently a linear or branched alkyl group of formula: C_nH_{2n+1} - in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom); a dibenzofuranyl group capable of having a substituent; and a dibenzothienyl group capable of having a substituent; the optional substituent of phenyl group, 9,9-dialkylfluorenyl group, dibenzofuranyl group and dibenzothienyl group is a fluorine atom or a linear or branched alkyl group of formula: C_nH_{2n+1} - in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom.

45 [0027] The present invention also provides an electroluminescence device, comprising: a pair of electrodes disposed on a substrate, and a luminescence unit comprising at least one organic compound disposed between the electrodes, wherein the organic compound comprises a metal coordination compound represented by the formula (1) described above.

50 [0028] In the luminescence device, a voltage is applied between the electrodes to emit light.

[0029] In a preferred embodiment of the electroluminescence device, a voltage is applied between the electrodes to emit phosphorescence.

[0030] The present invention further provides a picture display apparatus, comprising an electroluminescence device

described above and a means for supplying electric signals to the electroluminescence device.

[0031] These and other objects, features and advantages of the present invention will become more apparent upon a consideration of the following description of the preferred embodiments of the present invention taken in conjunction with the accompanying drawings.

5

BRIEF DESCRIPTION OF THE DRAWINGS

[0032]

10 Figures 1A, 1B and 1C illustrate embodiments of the luminescence device according to the present invention, respectively.

Figure 2 schematically illustrates a panel structure including an EL device and drive means.

DETAILED DESCRIPTION OF THE PREFERRED EMBODIMENTS

15

[0033] Basic structures of organic luminescence (EL) devices formed according to the present invention are illustrated in Figures 1A, 1B and 1C.

15 [0034] As shown in these figures, an organic luminescence device generally comprises, on a transparent substrate 15, a 50 to 200 nm-thick transparent electrode 14, a plurality of organic film layers and a metal electrode 11 formed so as to cover the organic layers.

20 [0035] Figure 1A shows an embodiment wherein the organic luminescence device comprises a luminescence layer 12 and a hole-transporting layer 13. The transparent electrode 14 may comprise ITO, etc., having a large work function so as to facilitate hole injection from the transparent electrode 14 to the hole-transporting layer 13. The metal electrode 11 comprises a metal material having a small work function, such as aluminum, magnesium or alloys of these elements, so as to facilitate electron injection into the organic luminescence device.

25 [0036] The luminescence layer 12 comprises a compound (metal coordination compound) according to the present invention. The hole-transporting layer 13 may comprise, e.g., a triphenylamine derivative, as represented by α -NPD mentioned above, and also a material having an electron-donative property as desired.

30 [0037] A device organized above exhibits a current-rectifying characteristic, and when an electric field is applied between the metal electrode 11 as a cathode and the transparent electrode 14 as an anode, electrons are injected from the metal electrode 11 into the luminescence layer 12, and holes are injected from the transparent electrode 15. The injected holes and electrons are recombined in the luminescence layer 12 to form excitons having high energy potential, which cause luminescence during transition to the ground state. In this instance, the hole-transporting layer 13 functions as an electron-blocking layer to increase the recombination efficiency at the boundary between the luminescence layer 12 and the hole-transporting layer 13, thereby providing an enhanced luminescence efficiency.

35 [0038] Further, in the structure of Figure 1B, an electron-transporting layer 16 is disposed between the metal electrode 11 and the luminescence layer 12 in Figure 1A. As a result, the luminescence function is separated from the functions of electron transportation and hole transportation to provide a structure exhibiting more effective carrier blocking, thus increasing the luminescence efficiency. The electron-transporting layer 16, may comprise, e.g., an oxadiazole derivative.

40 [0039] Figure 1C shows another desirable form of a four-layer structure, including a hole-transporting layer 13, a luminescence layer 12, an exciton diffusion prevention layer 17 and an electron-transporting layer 16, successively from the side of the transparent electrode 14 as the anode.

45 [0040] The luminescence materials used in the present invention are most suitably metal coordination compounds represented by the above-mentioned formulae (1) to (5), which are found to cause high-efficiency luminescence, retain high luminance for a long period and show little deterioration by current passage.

[0041] The metal coordination compound of the present invention emits phosphorescence, and its lowest excited state is believed to be an MLCT* (metal-to-ligand charge transfer) excited state or $\pi-\pi^*$ excited state in a triplet state, and phosphorescence is caused at the time of transition from such a state to the ground state.

50 [0042] Hereinbelow, methods for measurement of some properties and physical values described herein for characterizing the luminescence material of the present invention will be described.

[0043] (1) Judgment between phosphorescence and fluorescence

[0044] The identification of phosphorescence was effected depending on whether deactivation with oxygen was caused or not. A solution of a sample compound in chloroform after aeration with oxygen or with nitrogen is subjected to photoillumination to cause photo-luminescence. The luminescence is judged to be phosphorescence if almost no luminescence attributable to the compound is observed with respect to the solution aerated with oxygen but photo-luminescence is confirmed with respect to the solution aerated with nitrogen. The phosphorescence of all the compounds of the present invention has been confirmed by this method unless otherwise noted specifically.

[0045] (2) Phosphorescence yield (a relative quantum yield, i.e., a ratio of an objective sample's quantum yield Φ (sample) to a standard sample's quantum yield Φ (st)) is determined according to the following formula:

$$5 \quad \Phi(\text{sample})/\Phi(\text{st}) =$$

$$[\text{Sem}(\text{sample})/\text{labs}(\text{sample})]/[\text{Sem}(\text{st})/\text{labs}(\text{st})],$$

10 wherein labs(st) denotes an absorption coefficient at an excitation wavelength of the standard sample; Sem(st), a luminescence spectral areal intensity when excited at the same wavelength; labs(sample), an absorption coefficient at an excitation wavelength of an objective compound; and Sem(sample), a luminescence spectral areal intensity when excited at the same wavelength.

[0046] Phosphorescence yield values described herein are relative values with respect to a phosphorescence yield $\Phi = 1$ of Ir(ppy)₃ as a standard sample.

15 [0047] (3) A method of measurement of phosphorescence life is as follows.

[0048] A sample compound is dissolved in chloroform and spin-coated onto a quartz substrate in a thickness of ca. 0.1 μm and is exposed to pulsative nitrogen laser light at an excitation wavelength of 337 nm at room temperature by using a luminescence life meter (made by Hamamatsu Photonics K.K.). After completion of the excitation pulses, the decay characteristic of luminescence intensity is measured.

20 [0049] When an initial luminescence intensity is denoted by I_0 , a luminescence intensity after $t(\text{sec})$ is expressed according to the following formula with reference to a luminescence life $\tau(\text{sec})$:

$$I = I_0 \cdot \exp(-t/\tau).$$

25 [0050] The luminescence material (metal coordination compound) of the present invention exhibited high phosphorescence quantum yields of 0.11 to 0.9 and short phosphorescence lives of 0.1 to 40 μsec . A short phosphorescence life becomes a condition for causing little energy deactivation and exhibiting an enhanced luminescence efficiency. More specifically if the phosphorescence life is long, the number of triplet state molecules maintained for luminescence is increased, and the deactivation process is liable to occur, thus resulting in a lower luminescence efficiency particularly at the time of a high-current density. The material of the present invention has a relatively short phosphorescence life thus exhibiting a high phosphorescence quantum yield, and is therefore suitable as a luminescence material for an EL device.

30 [0051] As a result of various studies of ours, it has been found that an organic EL device using the metal coordination compound of the formula (1) as a principal luminescence material causes high-efficiency luminescence, retains high luminance for a long period and shows little deterioration by current passage.

35 [0052] In the formula (1) representing the metal coordination compound of the present invention, n may preferably 0 or 1, more preferably 0. Further, the partial structure ML'n may preferably comprise the aromatic group represented by the above-mentioned formula (5). In the formula (5), Y may preferably comprise C=O or CRR'. When Y is CRR' where R and R' are CH₃, the metal coordination compound of the formula (1) may preferably have no substituent. Particularly, when CyC1 is FL2 (appearing hereinafter) where R and R' are CH₃ and CyN1 is Pi, R1 to R4 (as substituents for Pi and FL2) may preferably be hydrogen atom at the same time.

40 [0053] In the present invention, by incorporating the aromatic group of the formula (5) into the metal coordination compound of the formula (1), it becomes possible to control an emission wavelength (particularly to provide a long emission wavelength). The presence of the aromatic group of the formula (5) is effective in enhancing a solubility of the metal coordination compound of the present invention in an organic solvent, thus facilitating a purification thereof by recrystallization or column chromatography. As a result, the metal coordination compound of the present invention is suitable as a luminescence material for the organic EL device.

45 [0054] Further, as shown in Examples appearing hereinafter, it has been substantiated that the metal coordination compound of the present invention exhibited an excellent stability in a continuous current passage test. This may be attributable to incorporation of the aromatic group of the formula (5) into the molecular structure of the metal coordination compound of the formula (1) according to the present invention. More specifically, a change in intermolecular interaction due to the introduction of the aromatic group of the formula (5) allows an intermolecular interaction of the metal coordination compound with, e.g., a host material to suppress formation of exciton associates causing thermal deactivation, thus reducing a quenching process thereby to improve phosphorescence yield and device characteristics.

50 [0055] The luminescence device according to the present invention may preferably be an electroluminescence device of the type wherein a layer of the metal coordination compound of the formula (1) is disposed between opposing two electrodes and a voltage is applied between the electrodes to cause luminescence, as shown in Figures 1A, 1B and 1C.

[0056] For the application to a display, a drive system using a thin-film transistor (TFT) drive circuit according to an active matrix-scheme may be used. Hereinbelow, an embodiment of using a device of the present invention in combination with an active matrix substrate is briefly described with reference to Figure 2.

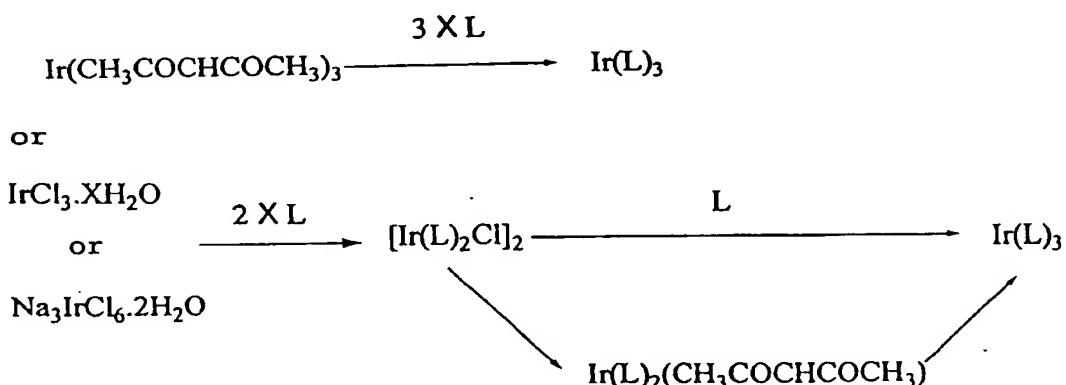
[0057] Figure 2 illustrates an embodiment of panel structure comprising an EL device and drive means. The panel is provided with a scanning signal driver, a data signal driver and a current supply source which are connected to gate selection lines, data signal lines and current supply lines, respectively. At each intersection of the gate selection lines and the data signal lines, a display pixel electrode is disposed. The scanning signal drive sequentially selects the gate selection lines G1, G2, G3 ... Gn, and in synchronism herewith, picture signals are supplied from the data signal driver to display a picture (image).

[0058] By driving a display panel including a luminescence layer comprising a luminescence material of the present invention, it becomes possible to provide a display which exhibits a good picture quality and is stable even for a long period display.

[0059] Some synthetic paths for providing a metal coordination compound represented by the above-mentioned formula (1) are illustrated below with reference to an iridium coordination compound ($m+n = 3$) for example:

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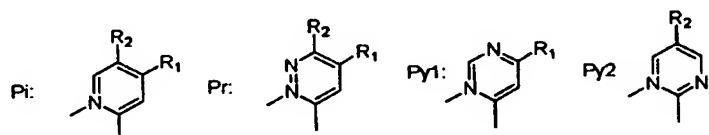
[0060] Other metal coordination compound ($M = Pt, Rh$ and Pd) can also be synthesized in a similar manner.

[0061] Some specific structural examples of metal coordination compounds used in the present invention are shown in Tables 1 to Tables 42 appearing hereinafter, which are however only representative examples and are not exhaustive.

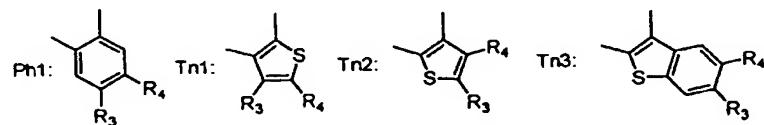
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Pi to Cz for CyN1, CyN2, CyC1 and CyC2 shown in Tables 1 to 42 represent partial structures shown below.

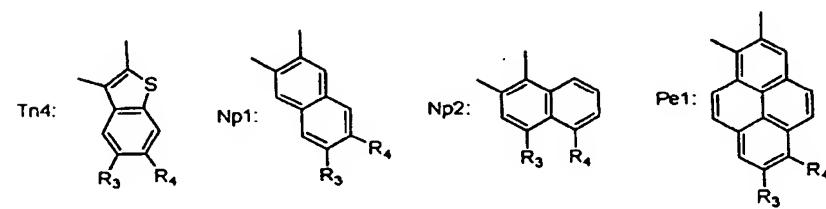
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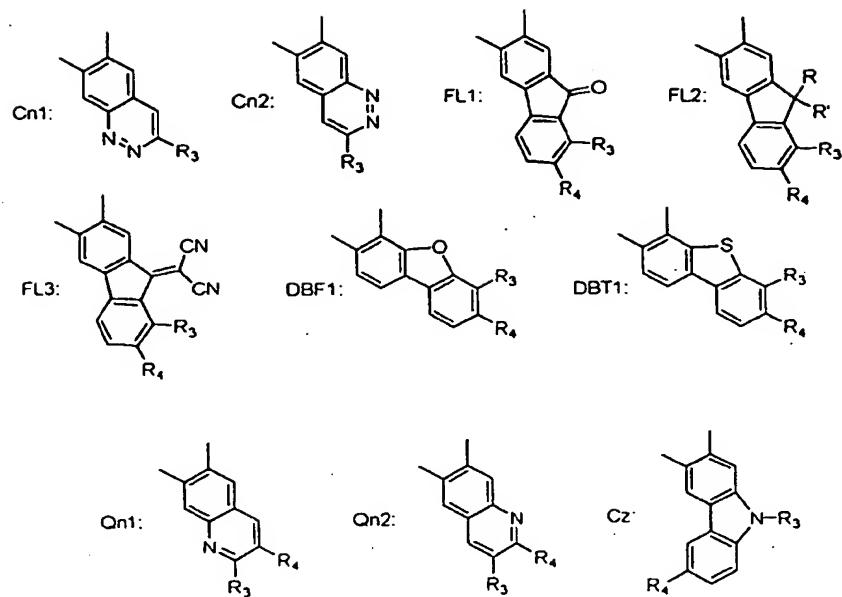
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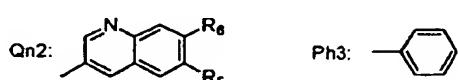
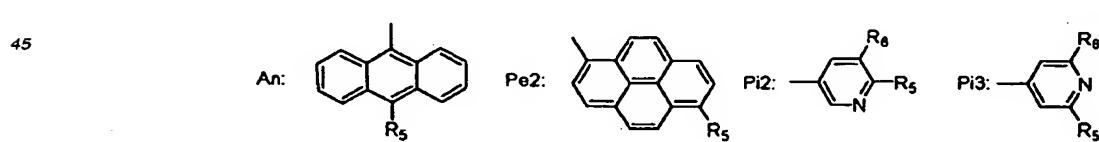
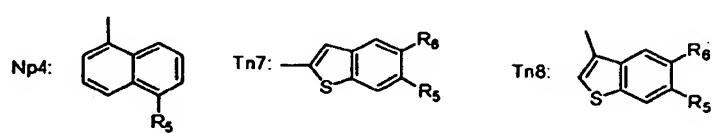
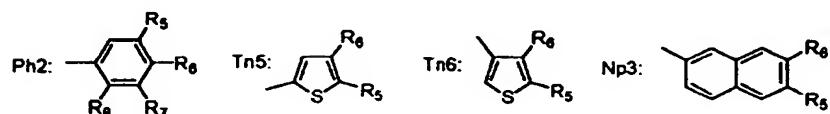
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EP 1 238 981 A2



[0062] Further, aromatic group Ph2 to DBT3 as substituents for CyN1, CyN2, CyC1 and CyC2 shown in Tables 1 to 42 represent partial structures shown below, with the proviso that substituents R5 to R8 of the aromatic groups represent hydrogen atoms when they are not specifically indicated.



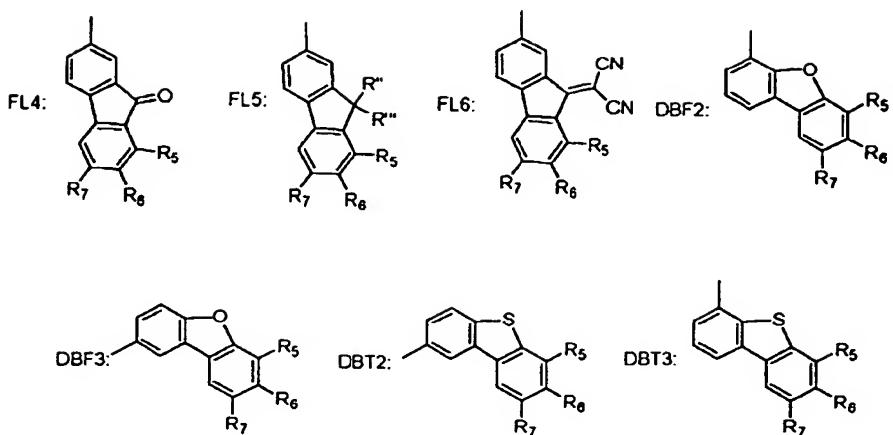


Table 1

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
1	Ir	3	0	Pi	FL1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
2	Ir	3	0	Pi	FL1	-	-	H	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
3	Ir	3	0	Pi	FL1	-	-	CF ₃	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
4	Ir	3	0	Pi	FL1	-	-	H	CH ₃	-	H	-	-
						-	-	H	H	-	-	-	-
5	Ir	3	0	Pi	FL1	-	-	H	H	-	-	-	-
						-	-	H	OC ₄ H ₉	-	-	-	-
6	Ir	3	0	Pi	FL1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
7	Ir	3	0	Pi	FL1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
8	Ir	3	0	Pi	FL1	-	-	H	FL6	H	H	H	-
						-	-	H	H	-	-	-	-
9	Ir	3	0	Pi	FL1	-	-	H	DBF2	H	H	H	-
						-	-	H	H	-	-	-	-
10	Ir	3	0	Pi	FL1	-	-	H	DBT3	H	H	H	-
						-	-	H	H	-	-	-	-
11	Ir	3	0	Pi	FL1	-	-	H	Ph2	H	H	H	H
						-	-	H	H	-	-	-	-

Table 1 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
5													
12	Ir	3	0	Pi	FL1	-	-	H	Ph2	H	C ₃ H ₇	H	H
10						-	-	H	H	-	-	-	-
13	Ir	3	0	Pi	FL1	-	-	H	FL4	H	Ph3	H	-
15						-	-	H	Ph2	H	H	H	H
14	Ir	3	0	Pi	FL1	-	-	H	Np4	H	-	-	-
20						-	-	H	H	-	-	-	-
15	Ir	3	0	Pi	FL1	-	-	H	Tn7	H	H	-	-
20						-	-	H	H	-	-	-	-
16	Ir	3	0	Pi	Ph1	-	-	H	FL4	H	H	H	-
25						-	-	H	H	-	-	-	-

Table 2

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
25													
17	Ir	3	0	Pi	Np2	-	-	H	FL4	H	H	H	-
30						-	-	H	H	-	-	-	-
18	Ir	3	0	Pi	FL1	-	-	H	Ph2	H	FL4	H	H
35						-	-	H	H	-	-	-	-
19	Ir	3	0	Pi	Ph1	-	-	H	H	-	-	-	-
40						-	-	FL4	H	H	H	H	-
20	Ir	3	0	Pi	Ph1	-	-	H	H	-	-	-	-
45						C ₂ H ₅	C ₂ H ₅	FL5	H	H	H	H	-
21	Ir	3	0	Pi	Ph1	-	-	H	Ph2	H	FL4	H	H
50						-	-	H	H	-	-	-	-
22	Ir	3	0	Pi	Np2	-	-	H	Ph2	H	FL4	H	H
55						-	-	H	H	-	-	-	-
23	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-
55						-	-	H	H	-	-	-	-
24	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-
55						-	-	H	H	-	-	-	-
25	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-
55						-	-	H	H	-	-	-	-

Table 2 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1							
										R''	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8
26	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	CH ₃	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-
27	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-	-	-
						-	-	H	OC ₄ H ₉	-	-	-	-	-	-	-	-
28	Ir	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	H	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-
29	Ir	3	0	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	H	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-
30	Ir	3	0	Pi	FL2	C ₄ H ₉	C ₄ H ₉	H	H	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-
31	Ir	3	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	H	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-
32	Ir	3	0	Pi	FL2	C ₆ H ₁₃	C ₆ H ₁₃	H	H	-	-	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-	-	-

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Table 3

No	M	m	n	CyN1	CyC1	R	R'	R"	CyC1-R3	CyN1-R1	CyN1-R2	CyN1		
												R5	R6	R7
33	Ir	3	0	Pi	FL2	C ₇ H ₁₅	C ₇ H ₁₅	H	H	H	-	-	-	-
34	Ir	3	0	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H	H	H	-	-	-	-
35	Ir	3	0	Pi	FL2	C ₁₀ H ₂₁	C ₁₀ H ₂₁	H	H	H	-	-	-	-
36	Ir	3	0	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	H	H	-	-	-	-
37	Ir	3	0	Pi	FL2	C ₂₀ H ₄₁	C ₂₀ H ₄₁	H	H	H	-	-	-	-
38	Ir	3	0	Pi	FL2	Ph3	Ph3	H	H	H	-	-	-	-
39	Ir	3	0	Pi	FL2	CH ₃	Ph3	H	H	H	-	-	-	-
40	Ir	3	0	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	H	H	-	-	-	-
41	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	H	-	-	-	-
42	Ir	3	0	Pi	FL2	H	H	H	H	H	H	H	H	H
43	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	H	H	H	H	H
						CH ₃	CH ₃	H	H	H	-	-	-	-

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Table 3 (continued)

No	M	m	n	CyN1	CyC1	R	R"	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
44	Ir	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H			FL5	H	H	-
45	Ir	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H			-	-	-	-
46	Ir	3	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H			FL5	H	H	-
47	Ir	3	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H			-	-	-	-
48	Ir	3	0	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H			FL5	H	H	-
						C ₁₅ H ₃₁	C ₁₅ H ₃₁	H				H	H	-
						C ₁₅ H ₃₁	C ₁₅ H ₃₁	H			-	-	-	-
						Ph3	Ph3	H			FL5	H	H	-
						Ph3	Ph3	H			-	-	-	-

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Table 4

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
49	Ir	3	0	Pi	FL2	CH ₃							R5	R6
50	Ir	3	0	Pi	FL2	(CH ₂) ₅ Ph ₃	Ph ₃	H	FL5	H	H	H	-	-
51	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	FL5	H	H	H	-	-
52	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	FL6	H	H	H	-	-
53	Ir	3	0	Pi	FL2	CH ₅	C ₂ H ₅	C ₂ H ₅	DBF2	H	H	H	-	-
54	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	DBT3	H	H	H	-	-
55	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	Ph2	H	H	H	-	-
56	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H	-
57	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	Ph2	H	OC≡C-C ₇ H ₁₅	H	H	-
58	Ir	3	0	Pi	FL2	C ₃ H ₇	C ₃ H ₇	C ₃ H ₇	Tn5	H	H	-	-	-
59	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	Tn6	H	H	-	-	-

Table 4 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
60	Ir	3	0	Pi	FL2	CH ₃					Np3	H	H	-
61	Ir	3	0	Pi	FL2	CH ₃		-	H	H	-	-	-	-
62	Ir	3	0	Pi	FL2	CH ₃		-	H	Np4	H	-	-	-
63	Ir	3	0	Pi	FL2	CH ₃		-	H	-	H	-	-	-
64	Ir	3	0	Pi	FL2	CH ₃		-	H	Tn7	H	H	-	-
									H	-	H	-	-	-

Table 5

No	M	m	n	CyN1	CyC1	R	R"	R'	CyN1-R1		CyC1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
65	Ir	3	0	Pi	FL2	CH ₃					Pe2	H	-	-
66	Ir	3	0	Pi	FL2	CH ₃	CH ₃		-	H	-	-	-	-
67	Ir	3	0	Pi	FL2	CH ₃			-	H	PI2	H	H	-
68	Ir	3	0	Pi	FL2	CH ₃	CH ₃		-	H	-	-	-	-
69	Ir	3	0	Pi	FL2	Ph3				Qn2	H	H	-	-
70	Ir	3	0	Pi	FL2	CH ₃	Ph3	H		H	-	-	-	-
71	Ir	3	0	Pi	FL2	CH ₃	CH ₃		-	H	-	-	-	-
72	Ir	3	0	Pi	FL2	CH ₃				H	FL4	H	Ph3	H
73	Ir	3	0	Pi	FL2	Ph3	Ph3	H		H	Ph2	H	H	H
74	Ir	3	0	Pi	FL2	CH ₃	Ph3	H		H	FL5	H	Ph3	H
75	Ir	3	0	Pi	FL2	CH ₃	Ph3	H		H	FL5	H	Ph3	H
						CH ₃	Ph3	H		H	Ph2	H	H	H

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Table 5 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
76	Ir	3	0	Pi	FL2	(CH ₂) ₃ Ph3	(CH ₂) ₃ Ph3	H	FL5	H	Ph3	H	-
77	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H
78	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
79	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Tn5	C ₃ H ₇	H	-	-
80	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Tn6	H	H	-	-
						CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Np3	H	H	-	-
						CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Np4	H	-	-	-

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Table 6

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
R'' R''' CyC1-R3 CyC1-R4													
81	Ir	3	0	Pi	FL2	CH ₃	Ph3	H	FL5	H	Ph3	H	-
						CH ₃	Ph3	H	Tn7	H	H	-	-
82	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Tn8	H	H	-	-
83	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	An	H	-	-	-
84	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Pe2	H	-	-	-
85	Ir	3	0	Pi	FL2	CH ₃	Ph3	H	FL5	H	Ph3	H	-
						CH ₃	Ph3	H	Pi2	C ₂ H ₅	H	-	-
86	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Pi3	H	H	-	-
87	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Qn2	H	H	-	-
88	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	DBT3	H	H	-	-
89	Ir	3	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
90	Ir	3	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						C ₅ H ₁₁	C ₅ H ₁₁	H	H	-	-	-	-
91	Ir	3	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	CF3	-	-	-	-
92	Ir	3	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						Ph3	Ph3	H	H	-	-	-	-
93	Ir	3	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						CH ₃	Ph3	H	H	-	-	-	-
94	Ir	3	0	Pi	Tn1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
95	Ir	3	0	Pi	Tn2	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
96	Ir	3	0	Pi	Tn3	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-

Table 7

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1												
										R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8					
CyC1																						
R5 R6 R7 R8																						
97	Ir	3	0	Pi	Tn4	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
98	Ir	3	0	Pi	Np1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
99	Ir	3	0	Pi	Np2	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
100	Ir	3	0	Pi	Pe1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
101	Ir	3	0	Pi	Np2	-	-	H	FL5	H	H	H	-									
						Ph3	Ph3	H	H	-	-	-	-									
102	Ir	3	0	Pi	Pe2	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
103	Ir	3	0	Pi	Cn1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	-	-	-	-	-									
104	Ir	3	0	Pi	Cn2	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	-	-	-	-	-									
105	Ir	3	0	Pi	FL3	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
106	Ir	3	0	Pi	DBF1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
107	Ir	3	0	Pi	DBT1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
108	Ir	3	0	Pi	Qn1	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
109	Ir	3	0	Pi	Qn2	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	H	H	-	-	-	-									
110	Ir	3	0	Pi	Cz	-	-	H	FL5	H	H	H	-									
						CH ₃	CH ₃	Ph3	H	-	-	-	-									
111	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	FL5	H	H									
						CH ₃	CH ₃	H	H	-	-	-	-									
112	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Tn5	FL5	H	-	-									
						CH ₃	CH ₃	H	H	-	-	-	-									

Table 8

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1											
										R5	R6	R7	R8								
CyC1																					
CyC1																					
113	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Tn6	FL5	H	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
114	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Np3	FL5	H	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
115	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Np4	FL5	-	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
116	Ir	3	0	Pi	FL2	Ph3	Ph3	H	Tn7	FL5	H	-	-								
						Ph3	Ph3	H	H	-	-	-	-								
117	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Tn8	FL5	H	-	-								
						Ph3	Ph3	H	H	-	-	-	-								
118	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	An	FL5	-	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
119	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Pe2	FL5	-	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
120	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Qn2	FL5	H	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
121	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL4	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
122	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
123	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL6	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
124	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	DBF2	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
125	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	DBF3	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
126	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	DBT2	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
127	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	DBT3	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
128	Ir	3	0	Pi	Ph1	-	-	H	H	-	-	-	-								
						C ₈ H ₁₇	C ₈ H ₁₇	FL5	H	H	H	H	-								

Table 9

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1							
										R''	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8
CyC1														R5	R6	R7	R8
129	Ir	3	0	Pi	Tn1	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
130	Ir	3	0	Pi	Tn2	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
131	Ir	3	0	Pi	Tn3	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
132	Ir	3	0	Pi	Tn4	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
133	Ir	3	0	Pi	Np2	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
134	Ir	3	0	Pi	Pe1	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
135	Ir	3	0	Pi	Cn1	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	-	H	H	H	-				
136	Ir	3	0	Pi	Cn2	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	-	H	H	H	-				
137	Ir	3	0	Pi	FL3	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
138	Ir	3	0	Pi	DBF1	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
139	Ir	3	0	Pi	DBT1	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
140	Ir	3	0	Pi	Qn1	-	-	H	H	-	-	-	-				
						CH ₃	Ph3	FL5	H	H	H	H	-				
141	Ir	3	0	Pi	Qn2	-	-	H	H	-	-	-	-				
						C ₅ H ₁₁	C ₅ H ₁₁	FL5	H	H	H	H	-				
142	Ir	3	0	Pi	Cz	-	-	H	H	-	-	-	-				
						CH ₃	CH ₃	FL5	H	H	H	H	-				
143	Ir	3	0	Pi	Ph1	-	-	H	Ph2	H	FL5	H	H				
						CH ₃	CH ₃	H	H	-	-	-	-				
144	Ir	3	0	Pi	FL3	-	-	H	H	-	-	-	-				
						-	-	H	H	-	-	-	-				

Table 10

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R""	CyC1-R3	CyC1-R4	Cyc1			
										R5	R6	R7	R8
145	Ir	3	0	Pi	FL3	-	-	H	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
146	Ir	3	0	Pi	DBF1	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
147	Ir	3	0	Pi	DBT1	CH ₃	CH ₃	H	CH ₃	-	-	-	-
						-	-	H	H	-	-	-	-
148	Ir	3	0	Pi	FL3	-	-	H	FL6	H	H	H	-
						-	-	H	H	-	-	-	-
149	Ir	3	0	Pi	DBF1	-	-	H	DBF2	H	H	H	-
						-	-	H	H	-	-	-	-
150	Ir	3	0	Pi	DBT1	-	-	H	DBT3	H	H	H	-
						-	-	H	H	-	-	-	-
151	Rh	3	0	Pi	FL1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
152	Rh	3	0	Pi	FL1	-	-	H	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
153	Rh	3	0	Pi	FL1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
154	Rh	3	0	Pi	FL1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
155	Rh	3	0	Pi	FL1	-	-	H	Ph2	H	H	H	H
						-	-	H	H	-	-	-	-
156	Rh	3	0	Pi	FL1	-	-	H	FL4	H	Ph3	H	-
						-	-	H	Ph2	H	H	H	H
157	Rh	3	0	Pi	FL1	-	-	H	Np4	H	-	-	-
						-	-	H	H	-	-	-	-
158	Rh	3	0	Pi	Ph1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
159	Rh	3	0	Pi	Np2	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
160	Rh	3	0	Pi	FL1	-	-	H	Ph2	H	FL4	H	H
						-	-	H	H	-	-	-	-

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Table 11

No	M	m	n	CyN1	CyC1	R	R"	R"	CyN1-R1	CyN1-R2	CyC1-R3	CyC1-R4	CyN1				
													R5	R6	R7	R8	
161	Rh	3	0	Pi	Ph1	-	-	-	H	H	-	-	-	-	-	-	
162	Rh	3	0	Pi	Ph1	-	-	-	FL4	H	H	H	-	-	-	-	
163	Rh	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	H	H	H	FL4	H	H	-	-	
164	Rh	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	H	H	H	-	-	-	-	-	
165	Rh	3	0	Pi	FL2	CH ₃	CH ₃	CH ₃	C ₂ H ₅	H	C ₂ H ₅	-	-	-	-	-	
166	Rh	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	C ₂ H ₅	H	H	H	-	-	-	-	-	
167	Rh	3	0	Pi	FL2	C ₃ H ₇	C ₃ H ₇	C ₃ H ₇	H	H	H	-	-	-	-	-	
168	Rh	3	0	Pi	FL2	C ₄ H ₉	C ₄ H ₉	C ₄ H ₉	H	H	H	-	-	-	-	-	
169	Rh	3	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	C ₅ H ₁₁	H	H	H	-	-	-	-	-	
170	Rh	3	0	Pi	FL2	C ₆ H ₁₃	C ₆ H ₁₃	C ₆ H ₁₃	H	H	H	-	-	-	-	-	
171	Rh	3	0	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	H	H	-	-	-	-	-	
						-	-	-	H	OC ₄ H ₉	-	-	-	-	-	-	-

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Table 11 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1	
									CyC1-R3	CyC1-R4	R5	R6
172	Rh	3	0	Pi	FL2	Ph3	Ph3	H	H	-	-	-
173	Rh	3	0	Pi	FL2	CH ₃	-	H	H	-	-	-
174	Rh	3	0	Pi	FL2	(CH ₂) ₃ Ph3	(CH ₂) ₅ Ph3	H	H	-	-	-
175	Rh	3	0	Pi	FL2	H	H	-	H	-	-	-
176	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	H	FL5	H	H
						CH ₃	CH ₃	H	H	-	-	-
						CH ₃	CH ₃	H	H	FL5	H	H
								H	H	-	-	-

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Table 12

No	M	m	n	CyN1	CyC1	R	R'	R''	CyN1-R1		CyN1-R2		CyN1		
									CyC1-R3	CyC1-R4	CyC1	R5	R6	R7	R8
177	Rh	3	0	Pi	FL2	C ₂ H ₆	C ₂ H ₅	H	FL5	H	H	H	-	-	-
178	Rh	3	0	Pi	FL2	C ₃ H ₁₁	C ₅ H ₁₁	H	FL5	H	H	H	-	-	-
179	Rh	3	0	Pi	FL2	CH ₃	C ₅ H ₁₁	H	FL5	H	H	H	-	-	-
180	Rh	3	0	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H	FL5	H	H	H	-	-	-
181	Rh	3	0	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	FL5	H	H	H	-	-	-
182	Rh	3	0	Pi	FL2	CH ₃	Ph3	H	FL5	H	H	H	-	-	-
183	Rh	3	0	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	FL5	H	H	H	-	-	-
184	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	FL6	H	H	H	-	-	-
185	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	-	-	-
186	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	CF ₃	H	H	-	-	-
187	Rh	3	0	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	Tn5	H	H	H	-	-	-

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Table 12 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
188	Rh	3	0	Pi	FL2	CH ₃	CH ₃	-	H	Np3	H	H	-	-
189	Rh	3	0	Pi	FL2	CH ₃	CH ₃	-	H	Np4	H	-	-	-
190	Rh	3	0	Pi	FL2	CH ₃	CH ₃	-	H	Tn8	H	H	-	-
191	Rh	3	0	Pi	FL2	CH ₃	CH ₃	-	H	An	H	-	-	-
192	Rh	3	0	Pi	FL2	CH ₃	CH ₃	-	H	Pe2	H	-	-	-

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Table 13

No	M	m	n	CyN1	CyC1	R	R"	R'	R"	CyN1-R1		CyC1-R2		CyN1	
										CyC1-R3	CyC1-R4	R5	R6	R7	R8
193	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	FL4	H	Ph3	H	-		
194	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H		
195	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-		
196	Rh	3	0	Pi	FL2	CH ₃	Ph3	Ph3	Ph2	H	H	H	H		
197	Rh	3	0	Pi	FL2	(CH ₂) ₃ Ph3	(CH ₂) ₃ Ph3	H	FL5	H	Ph3	H	-		
198	Rh	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H		
199	Rh	3	0	Pi	Ph1	-	-	H	Tn5	C ₃ H ₇	H	-	-		
200	Rh	3	0	Pi	Ph1	CH ₃	CH ₃	H	FL5	H	H	H	H		
201	Rh	3	0	Pi	Ph1	C ₅ H ₁₁	C ₅ H ₁₁	H	-	-	-	-	-		
202	Rh	3	0	Pi	Tn4	-	-	H	FL5	H	H	H	H		
203	Rh	3	0	Pi	Np2	-	-	H	FL5	H	H	H	H		
						CH ₃	CH ₃	H	-	-	-	-	-		

Table 13 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R''	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
204	Rh	3	0	Pi	Fl2	CH ₃					Ph2	H	Fl5	H
205	Rh	3	0	Pi	Fl2	CH ₃	CH ₃	CH ₃	H	H	-	-	-	-
206	Rh	3	0	Pi	Fl2	CH ₃	CH ₃	CH ₃	H	Tn5	Fl5	H	-	-
207	Rh	3	0	Pi	Fl2	CH ₃	CH ₃	CH ₃	H	H	-	-	-	-
208	Rh	3	0	Pi	Ph1	-					H	H	-	-
						C ₈ H ₁₇	C ₈ H ₁₇	FL5	H	H	H	H	H	-

Table 14

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
										CyC1			
										R5	R6	R7	R8
209	Rh	3	0	Pi	Tn1	-	-	H	H	-	-	-	-
						CH ₃	CH ₃	FL5	H	H	H	H	-
210	Rh	3	0	Pi	Ph1	-	-	H	Ph2	H	FL5	H	H
						CH ₃	CH ₃	H	H	-	-	-	-
211	Pt	2	0	Pi	FL1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
212	Pt	2	0	Pi	FL1	-	-	H	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
213	Pt	2	0	Pi	FL1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
214	Pt	2	0	Pi	FL1	-	-	H	DBT3	H	H	H	-
						-	-	H	H	-	-	-	-
215	Pt	2	0	Pi	FL1	-	-	H	Ph2	H	H	H	H
						-	-	H	H	-	-	-	-
216	Pt	2	0	Pi	FL1	-	-	H	FL4	H	Ph3	H	-
						-	-	H	Ph2	H	H	H	H
217	Pt	2	0	Pi	FL1	-	-	H	Np4	H	-	-	-
						-	-	H	H	-	-	-	-
218	Pt	2	0	Pi	Ph1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
219	Pt	2	0	Pi	Np2	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
220	Pt	2	0	Pi	FL1	-	-	H	Ph2	H	FL4	H	H
						-	-	H	H	-	-	-	-
221	Pt	2	0	Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	FL4	H	H	H	H	-
222	Pt	2	0	Pi	Ph1	-	-	H	H	-	-	-	-
						C ₂ H ₅	C ₂ H ₅	FL5	H	H	H	H	-
223	Pt	2	0	Pi	Np2	-	-	H	Ph2	H	FL4	H	H
						-	-	H	H	-	-	-	-
224	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

Table 15

No	M	m	n	CyN1	CyC1	R	R"	R"	CyC1-R3	CyN1-R1	CyC1-R4	CyN1			
												R5	R6	R7	R8
225	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-	-	-
226	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-	-	-
227	Pt	2	0	Pi	FL2	Ph3	Ph3	H	H	-	-	-	-	-	-
228	Pt	2	0	Pi	FL2	CH ₃	Ph3	H	H	-	-	-	-	-	-
229	Pt	2	0	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	H	-	-	-	-	-	-
230	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	H	H	-	-
231	Pt	2	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	FL5	H	H	H	H	-	-
232	Pt	2	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	H	-	-	-	-	-	-
233	Pt	2	0	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H	FL5	H	H	H	H	-	-
234	Pt	2	0	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	FL5	H	H	H	H	-	-
235	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H	-	-

Table 15 (continued)

No	M	m	n	CyN1	Cyc1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
236	Pt	2	0	Pi	FL2	CH ₃			H	Ph2	CF ₃	H	H	H
237	Pt	2	0	Pi	FL2	CH ₃		-	H	H	-	-	-	-
238	Pt	2	0	Pi	FL2	CH ₃		-	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H
239	Pt	2	0	Pi	FL2	CH ₃		-	H	H	-	-	-	-
240	Pt	2	0	Pi	FL2	CH ₃		-	H	FL4	H	Ph3	H	-
										Ph2	H	H	H	H

Table 16

No	M	m	n	CyN1	CyC1	R	R'	R''	R'''	CyN1-R1		CyN1-R2		CyN1	
										CyC1-R3	CyC1-R4	R5	R6	R7	R8
241	Pt	2	0	Pi	FL2	CH ₃	CH ₃	CH ₃	H	FL5	H	Ph3	H	-	
242	Pt	2	0	Pi	FL2	Ph3	Ph3	CH ₃	H	Ph2	H	H	H	H	
243	Pt	2	0	Pi	FL2	(CH ₂) ₃ Ph3	(CH ₂) ₃ Ph3	CH ₃	H	FL5	H	Ph3	H	-	
244	Pt	2	0	Pi	FL2	CH ₃	CH ₃	CH ₃	H	Ph2	H	H	H	H	
245	Pt	2	0	Pi	FL2	CH ₃	CH ₃	CH ₃	H	FL5	H	Ph3	H	-	
246	Pt	2	0	Pi	Ph1	-	-	CH ₃	H	Tn5.	C ₃ H ₇	H	-	-	
247	Pt	2	0	Pi	Ph1	-	-	CH ₃	H	FL5	H	Ph3	H	-	
248	Pt	2	0	Pi	Ph1	C ₅ H ₁₁	-	CH ₃	H	FL5	H	H	H	-	
249	Pt	2	0	Pi	Ph1	-	-	C ₅ H ₁₁	H	FL5	H	H	H	-	
250	Pt	2	0	Pi	Ph1	Ph3	Ph3	CH ₃	H	FL5	H	H	H	-	
251	Pt	2	0	Pi	Tn1	-	-	CH ₃	H	FL5	H	H	H	-	

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Table 16 (continued)

No	M	m	n	Cyn1	CyC1	R	R'	R''	Cyn1-R1		Cyn1-R2		Cyn1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
252	Pt	2	0	Pi	Np2	-	-	H	FL5	H	H	H	-	-
253	Pt	2	0	Pi	Pe2	-	-	H	FL5	H	H	H	-	-
254	Pt	2	0	Pi	Cn1	-	-	H	FL5	H	H	H	-	-
255	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	-	-	-	-	-	-
256	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	Tn5	FL5	H	-	-	-
						CH ₃	CH ₃	H	H	-	-	-	-	-

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Table 17

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1											
										R5	R6	R7	R8								
CyC1																					
CyC1																					
257	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	Tn6	FL5	H	-	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
258	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	FL4	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
259	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	FL5	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
260	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	FL6	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
261	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	DBF2	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
262	Pt	2	0	Pi	FL2	CH ₃	CH ₃	H	DBF3	FL5	H	H	-								
						CH ₃	CH ₃	H	H	-	-	-	-								
263	Pt	2	0	Pi	Ph1	-	-	H	H	-	-	-	-								
						C ₈ H ₁₇	C ₈ H ₁₇	FL5	H	H	H	H	-								
264	Pt	2	0	Pi	Tn1	-	-	H	H	-	-	-	-								
						CH ₃	CH ₃	FL5	H	H	H	H	-								
265	Pt	2	0	Pi	Tn2	-	-	H	H	-	-	-	-								
						CH ₃	CH ₃	FL5	H	H	H	H	-								
266	Pt	2	0	Pi	Ph1	-	-	H	Ph2	H	FL5	H	H								
						CH ₃	CH ₃	H	H	-	-	-	-								
267	Pt	2	0	Pi	FL3	-	-	H	H	-	-	-	-								
						-	-	H	H	-	-	-	-								
268	Pt	2	0	Pi	FL3	-	-	H	CF ₃	-	-	-	-								
						-	-	H	H	-	-	-	-								
269	Pt	2	0	Pi	DBF1	-	-	CF ₃	CF ₃	-	-	-	-								
						-	-	H	H	-	-	-	-								
270	Pt	2	0	Pi	DBT1	-	-	H	CH ₃	-	-	-	-								
						-	-	H	H	-	-	-	-								
271	Pd	2	0	Pi	FL1	-	-	H	H	-	-	-	-								
						-	-	H	H	-	-	-	-								
272	Pd	2	0	Pi	FL1	-	-	H	CF ₃	-	-	-	-								
						-	-	H	H	-	-	-	-								

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Table 18

No	M	m	n	C _y N1	C _y C1	R	R'	R ^{III}	C _y C1-R1	C _y N1-R2	C _y N1					
											C _y C1-R3	C _y C1-R4	R5	R6	R7	R8
273	Pd	2	0	Pi	FL1	-	-	H	FL4	H	H	H	-	-	-	-
274	Pd	2	0	Pi	FL1	-	-	H	H	-	-	-	-	-	-	-
275	Pd	2	0	Pi	FL1	-	-	H	Ph2	H	H	H	H	H	H	H
276	Pd	2	0	Pi	FL1	-	-	H	FL4	H	Ph3	H	-	-	-	-
277	Pd	2	0	Pi	Ph1	-	-	H	Ph2	H	H	H	H	H	H	H
278	Pd	2	0	Pi	Np2	-	-	H	Np4	H	-	-	-	-	-	-
279	Pd	2	0	Pi	FL1	-	-	H	FL4	H	H	H	H	H	H	H
280	Pd	2	0	Pi	Ph1	-	-	H	FL4	H	H	H	H	H	H	H
281	Pd	2	0	Pi	Np2	-	-	H	Ph2	H	FL4	H	H	H	H	H
282	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-	-
283	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	H	CF ₃	-	-	-	-	-	-

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Table 18 (continued)

No	M	m	n	CyN1	CyC1	R	R"	R"	CyN1-R1		CyN1	
									CyC1-R3	CyC1-R4	R5	R6
284	Pd	2	0	Pi	FL2	(CH ₂) ₅ Ph ₃	(CH ₂) ₅ Ph ₃	H	H	-	-	-
285	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-
286	Pd	2	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	FL5	H	H	H
287	Pd	2	0	Pi	FL2	(CH ₂) ₅ Ph ₃	(CH ₂) ₅ Ph ₃	H	FL5	H	H	H
288	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H

Table 19

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'"	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
289	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	CF ₃	H	H	H
						-	-	H	H	-	-	-	-
290	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	FL4	H	Ph3	H	-
						-	-	H	Ph2	H	H	H	H
291	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Ph2	H	H	H	H
292	Pd	2	0	Pi	FL2	Ph3	Ph3	H	FL5	H	Ph3	H	-
						Ph3	Ph3	H	Ph2	H	H	H	H
293	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	DBT3	H	H	-	-
294	Pd	2	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
295	Pd	2	0	Pi	Ph1	-	-	H	FL5	H	H	H	-
						C ₅ H ₁₁	C ₅ H ₁₁	H	H	-	-	-	-
296	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	FL5	H	H
						CH ₃	CH ₃	H	H	-	-	-	-
297	Pd	2	0	Pi	FL2	CH ₃	CH ₃	H	Tn5	FL5	H	-	-
						CH ₃	CH ₃	H	H	-	-	-	-
298	Pd	2	0	Pi	Ph1	-	-	H	H	-	-	-	-
						C ₈ H ₁₇	C ₈ H ₁₇	FL5	H	H	H	H	-
299	Pd	2	0	Pi	Ph1	-	-	H	Ph2	H	FL5	H	H
						CH ₃	CH ₃	H	H	-	-	-	-
300	Pd	2	0	Pi	DBT1	-	-	H	CH ₃	-	-	-	-
						-	-	H	H	-	-	-	-

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Table 20

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1															
										R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8								
CyC1													CyC1												
CyN2													CyN2												
CyC2													CyC2												
R5 R6 R7 R8													R5 R6 R7 R8												
R5 R6 R7 R8													R5 R6 R7 R8												
R5 R6 R7 R8													R5 R6 R7 R8												
R5 R6 R7 R8													R5 R6 R7 R8												
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R5 R6 R7 R8																									

EP 1 238 981 A2

Table 20 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1				
										R5	R6	R7	R8	
5						R"	R'"	CyC1-R3	CyC1-R4	CyC1				
										R5	R6	R7	R8	
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2				
10										R5	R6	R7	R8	
						R"	R'''	CyC2-R3	CyC2-R4	CyC2				
										R5	R6	R7	R8	
15	308	Ir	2	1	Pi	FL1	-	-	H	Ph2	H	FL4	H	H
							-	-	H	H	-	-	-	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
20	309	Ir	2	1	Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	FL4	H	H	H	H	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
25	310	Ir	2	1	Pi	Ph1	-	-	H	Ph2	H	FL4	H	H
							-	-	H	H	-	-	-	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
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Table 21

No	M	m	n	CyN1	Cyc1	R	R'	R ^{III}	CyC1-R3	CyN1-R1	CyN1-R2	CyN1			
												R5	R6	R7	R8
311	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
312	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
313	Ir	2	1	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
314	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-
				Pi	Ph1	-	-	H	OC ₄ H ₉	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-

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Table 21 (continued)

No	M	m	n	C _y N1	C _y C1	R	R'	R ^{III}	C _y N1-R1		C _y N1-R2		C _y N1		
									C _y C1-R3	C _y C1-R4	R5	R6	R7	R8	
											R5	R6	R7	R8	
				C _y N2	C _y C2	R	R'		C _y N2-R1	C _y N2-R2					
								R ^{IV}	R ^V	C _y C2-R3	C _y C2-R4	R5	R6	R7	R8
												C _y C2			
315	Ir	2	1	Pi	Fl2	C ₈ H ₁₇	C ₈ H ₁₇		H	H	-	-	-	-	
				Pi	Ph1	-	-		H	H	-	-	-	-	
316	Ir	2	1	Pi	Fl2	Ph3	Ph3		H	H	-	-	-	-	
				Pi	Ph1	-	-		H	H	-	-	-	-	
317	Ir	2	1	Pi	Fl2	CH ₃	Ph3		H	H	-	-	-	-	
				Pi	Ph1	-	-		H	H	-	-	-	-	
318	Ir	2	1	Pi	Fl2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3		H	H	-	-	-	-	
				Pi	Ph1	-	-		H	H	-	-	-	-	
									H	H	-	-	-	-	

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Table 21 (continued)

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
										CyN2			
								CyN2-R1	CyN2-R2	CyN2			
										R5	R6	R7	R8
						R"	R'''	CyC2-R3	CyC2-R4	CyC2			
										R5	R6	R7	R8
319	Ir	2	1	Pi	FL2	H	H						
						CH ₃	CH ₃	H	H	FL5	H	H	-
				Pi	Ph1	-	-	H	H		-	-	-
						-	-	H	H		-	-	-
320	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	H	FL5	H	H	-
						CH ₃	CH ₃	H	H		-	-	-
				Pi	Ph1	-	-	H	H		-	-	-
						-	-	Cl	Cl		-	-	-

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Table 22

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1		CyN1-R2		CyN1			
								R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8
321	Ir	2	1	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H		FL5	H	H	H	-	
						C ₂ H ₅	C ₂ H ₅	H			-	-	-	-	
				Pr	Ph1	-	-	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	
322	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H		Ph2	H	H	R6	R7	R8
						-	-	H	H	-	-	-	-	-	
				Pr	Ph1	-	-	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	
323	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H		Ph2	H	OCH ₂ C ₅ F ₁₁	H	H	
						-	-	H	H	-	-	-	-	-	
				Py1	Ph1	-	-	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	
324	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H		Ph2	H	OC≡C-C ₇ H ₁₅	H	H	
						-	-	H	H	-	-	-	-	-	
				Py2	Ph1	-	-	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	

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Table 22 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R''	CyN1-R1		CyN1	
									R5	R6	R7	R8
									CyC1-R3	CyC1-R4		CyC1
											R5	R6
											R7	R8
									CyN2-R1	CyN2-R2		CyN2
											R5	R6
									CyC2-R3	CyC2-R4		CyC2
											R5	R6
											R7	R8
325	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H
						CH ₃	CH ₃	H	Ph2	H	H	H
				Pi	Ph1	-	H	H	-	-	-	-
						-	-	CH ₃	H	-	-	-
326	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H
						CH ₃	CH ₃	H	Tn8	H	H	-
				Pi	Ph1	-	H	H	-	-	-	-
						-	-	Br	H	-	-	-
327	Ir	2	1	Pi	Ph1	-	H		FL5	H	H	H
						CH ₃	CH ₃	H	H	-	-	-
				Pi	Ph1	-	H			-	-	-
						-	-			-	-	-
328	Ir	2	1	Pi	Ph1	-	H		CF ₃	H	-	-
						-	-			-	-	-
									FL5	H	H	H
				Pi	Ph1	-	H		H	-	-	-
						-	-		C ₅ H ₁₁	H	-	-

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Table 22 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	
				R"	R'"	CyC1-R3	CyC1-R4				R6	R7	R8
										R5	R6	R7	R8
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2				
										R5	R6	R7	R8
						R"	R'''	CyC2-R3	CyC2-R4				
										R5	R6	R7	R8
329	Ir	2	1	Pi	Np2	-	-	H	FL5	H	H	H	-
				Pi	Ph1			Ph3	H	H	-	-	-
						-	-	H	H	-	-	-	-
								OCH ₃	H	-	-	-	-
330	Ir	2	1	Pi	Fl2	CH ₃	CH ₃	Ph2	H	FL5	H	H	
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	Cl	H	-	-	-	-

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Table 23

No	M	m	n	CyN1	Cyc1	R	R"	R'	CyN1-R1		CyN1-R2		CyN1		
									CyC1-R3	CyC1-R4	CyC1	R5	R6	R7	R8
331	Ir	2	1	Pi	Fl2	CH ₃									
						-	-		H	H	-	-	-	-	-
				Pi	Tn1	-	-		H	H	-	-	-	-	-
332	Ir	2	1	Pi	Fl2	CH ₃	CH ₃	CF ₃							
				Pi	Tn1	-	-	H	H	H	-	-	-	-	-
333	Ir	2	1	Pi	Fl2	CH ₃	CH ₃	H							
				Pi	Tn2	-	-	H	H	H	-	-	-	-	-
334	Ir	2	1	Pi	Fl2	C ₄ H ₉	C ₄ H ₉	H							
				Pi	Tr3	-	-	H	H	H	-	-	-	-	-
						-	-	H	CH ₃	-	-	-	-	-	-

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Table 23 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1	CyN1-R2	CyN1			
											R5	R6	R7	R8
									CyC1-R3	CyC1-R4	CyC1			
											R5	R6	R7	R8
				CyN2	CyC2	R	R'	R"	CyN2-R1	CyN2-R2	CyN2			
											R5	R6	R7	R8
									CyC2-R3	CyC2-R4	CyC2			
											R5	R6	R7	R8
335	Ir	2	1	Pi	FL2	C ₈ H ₁₇	H	H	-	-	-	-	-	-
				Pi	Tn4	-	-	H	H	-	-	-	-	-
						-	-	H	H	-	-	-	-	-
336	Ir	2	1	Pi	FL2	H	H	H	FL5	H	H	H	-	-
				Pi	Np1	CH ₃	CH ₃	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-
337	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	H	-	-
				Pi	Np2	CH ₃	CH ₃	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-
338	Ir	2	1	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	FL5	H	H	H	-	-
				Pi	Po1	-	-	H	-	-	-	-	-	-
						-	-	H	-	-	-	-	-	-

Table 23 (continued)

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
				R"		R"	CyC1-R3	CyC1-R4	CyC1				
										R5	R6	R7	R8
							CyN2-R1	CyN2-R2	CyN2				
										R5	R6	R7	R8
							R"	R'''	CyC2-R3	CyC2-R4	CyC2		
										R5	R6	R7	R8
339	Ir	2	1	Pi	Fl2	CH ₃	Ph3	H	Fl5	H	H	H	-
						CH ₃	Ph3	H		-	-	-	-
				Pi	Cn1	-	-	H		-	-	-	-
340	Ir	2	1	Pi	Fl2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	Fl5	H	H	H	-
						CH ₃	CH ₃	H		-	-	-	-
				Pi	Cn2	-	-	H		-	-	-	-
								H		-	-	-	-

Table 24

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1		
										R5	R6	R7
				R"	R'''	CyC1-R3	CyC1-R4	CyC1			R8	
										R5	R6	R7
								CyN2-R1	CyN2-R2	CyN2		
										R5	R6	R7
										R8		
											CyC2	
341	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	DBT3	H	H	-
						-	-	H	-	-	-	-
				Pi	FL1	-	-	H	-	-	-	-
						-	-	H	-	-	-	-
342	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H
						-	-	H	-	-	-	-
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-
						-	-	H	-	-	-	-
343	Ir	2	1	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	Tn5	H	H	-
						-	-	H	-	-	-	-
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-
						-	-	H	-	-	-	-
344	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Np3	H	H	-
						-	-	H	-	-	-	-
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-
						-	-	H	-	-	-	-

Table 24 (continued)

No	M	m	n	C _y N1	C _y C1	R	R'	R''	C _y N1-R1		C _y N1	
									R5	R6	R7	R8
									C _y C1-R3	C _y C1-R4		C _y C1
											R5	R6
				C _y N2	C _y C2	R	R'		C _y N2-R1	C _y N2-R2		C _y N2
											R5	R6
									C _y C2-R3	C _y C2-R4		C _y C2
											R5	R6
345	Ir	2	1	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇		H	H	-	-
										H	H	-
				Pi	FL2	(CH ₂) ₅ Rh ₃	(CH ₂) ₅ Ph ₃		H	H	-	-
										H	H	-
346	Ir	2	1	Pi	FL2	Ph ₃	Ph ₃		H	H	-	-
										H	H	-
				Pi	FL2	C ₃ H ₇	C ₃ H ₇		H	H	-	-
										H	H	-
347	Ir	2	1	Pi	FL2	CH ₃	Ph ₃		H	H	-	-
										H	H	-
				Pi	FL3	-	-		H	H	-	-
										H	H	-
348	Ir	2	1	Pi	FL2	(CH ₂) ₅ Ph ₃	(CH ₂) ₅ Ph ₃		H	H	-	-
										H	H	-
				Pi	DBF1	-	-		H	H	-	-
										H	H	-

Table 24 (continued)

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Table 25

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R"	Cyc1-R3	Cyc1-R4				
										R5	R6	R7	R8
				CyN2	Cyc2	R	R'	CyN2-R1	CyN2-R2				
										R5	R6	R7	R8
						R"	R"	Cyc2-R3	Cyc2-R4				
										R5	R6	R7	R8
351	Ir	2	1	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	FL5	H	H	H	-
						C ₂ H ₅	C ₂ H ₅	H	-	-	-	-	-
				Pr	Qn2	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
352	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H
						-	-	H	-	-	-	-	-
				Pr	Cz	-	-	H	H	-	-	-	-
						-	-	Ph3	H	-	-	-	-
353	Rh	2	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
354	Rh	2	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OC≡C-C ₇ H ₁₅	H	H
						-	-	H	H	-	-	-	-
				Py2	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

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Table 25 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R''							
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2				
										R5	R6	R7	R8
						R''	R'''	CyC2-R3	CyC2-R4				
										R5	R6	R7	R8
355	Rh	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
				Pi	Ph1	-	-	H	H	H	H	H	H
						-	-	CH ₃	H	-	-	-	-
356	Rh	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
				Pi	Ph1	-	-	H	H	H	H	H	H
						-	-	Br	H	-	-	-	-
357	Rh	2	1	Pi	Ph1	-	-	H	Tn8	H	H	H	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						CH ₃	CH ₃	H	FL5	H	H	H	-
358	Rh	2	1	Pi	Ph1	-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	CF ₃	H	-	-	-	-
						-	-	H	FL5	H	H	H	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	C ₅ H ₁₁	H	-	-	-	-

Table 25 (continued)

Table 26

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1															
										R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8								
CyC1													R5	R6	R7	R8									
CyN2													R5	R6	R7	R8									
CyN2													R5	R6	R7	R8									
CyC2													R5	R6	R7	R8									
361	Ir	1	2	Pi	FL1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
362	Ir	1	2	Pi	FL1	-	-	H	FL4	H	H	H	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
363	Ir	1	2	Pi	FL1	-	-	H	Ph2	H	H	H	H	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
364	Ir	1	2	Pi	FL1	-	-	H	FL4	H	Ph3	H	-	-	-	-									
						-	-	H	Ph2	H	H	H	H	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
365	Ir	1	2	Pi	FL1	-	-	H	Np4	H	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
366	Ir	1	2	Pi	Ph1	-	-	H	FL4	H	H	H	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
367	Ir	1	2	Pi	Np2	-	-	H	FL4	H	H	H	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	-									
						-	-	H	H	-	-	-	-	-	-	-									

Table 26 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1				
										R5	R6	R7	R8	
5						R"	R'''	CyC1-R3	CyC1-R4	CyC1				
										R5	R6	R7	R8	
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2				
10				/						R5	R6	R7	R8	
						R"	R'''	CyC2-R3	CyC2-R4	CyC2				
										R5	R6	R7	R8	
15	368	Ir	1	2	Pi	FL1	-	-	H	Ph2	H	FL4	H	H
							-	-	H	H	-	-	-	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
20	369	Ir	1	2	Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	FL4	H	H	H	H	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
25	370	Ir	1	2	Pi	Ph1	-	-	H	Ph2	H	FL4	H	H
							-	-	H	H	-	-	-	-
					Pi	Ph1	-	-	H	H	-	-	-	-
							-	-	H	H	-	-	-	-
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Table 27

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
371	Ir	1	2	Pi	Fl2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
372	Ir	1	2	Pi	Fl2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
373	Ir	1	2	Pi	Fl2	CH ₃	CH ₃	C _F ₃	C _F ₃	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
374	Ir	1	2	Pi	Fl2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-

Table 27 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R''	R'''	CyN1-R1		CyN1-R2		CyN1		
										CyC1-R3	CyC1-R4	R5	R6	R7	R8	
				CyN2	CyC2	R	R'	R''	R'''	CyN2-R1	CyN2-R2	R5	R6	R7	R8	
												R5	R6	R7	R8	
										CyC2-R3	CyC2-R4	R5	R6	R7	R8	
												CyC2				
													R5	R6	R7	R8
375	Ir	1	2	Pi	Fl2	C ₈ H ₁₇	C ₈ H ₁₇	H	H	-	-	-	-	-	-	
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	
376	Ir	1	2	Pi	Fl2	Ph3	Ph3	H	H	-	-	-	-	-	-	
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	
377	Ir	1	2	Pi	Fl2	CH ₃	Ph3	H	H	-	-	-	-	-	-	
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	
378	Ir	1	2	Pi	Fl2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	H	-	-	-	-	-	-	
				Pi	Ph1	-	-	H	H	-	-	-	-	-	-	

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Table 27 (continued)

No	M	m	n	C _y N1	C _y C1	R	R'	C _y N1-R1	C _y N1-R2	C _y N1			
										R5	R6	R7	R8
						R"	R"	C _y C1-R3	C _y C1-R4	C _y C1			
										R5	R6	R7	R8
				C _y N2	C _y C2	R	R'	C _y N2-R1	C _y N2-R2	C _y N2			
										R5	R6	R7	R8
						R"	R"	C _y C2-R3	C _y C2-R4	C _y C2			
										R5	R6	R7	R8
379	Ir	1	2	Pi	Fl2	H	H			Fl5	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
380	Ir	1	2	Pi	Fl2	CH ₃	CH ₃	H	Fl5	H	H	-	-
						CH ₃	CH ₃	H	-	-	-	-	-
				Pi	Ph1	-	-	H	-	-	-	-	-
						-	-	Cl	H	-	-	-	-

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Table 28

No	M	m	n	CyN1	Cyc1	R	R'	R''	R'''	CyN1-R1	CyN1-R2	CyN1			
										Cyc1-R3	Cyc1-R4	R5	R6	R7	R8
381	Ir	1	2	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	FL5	H	H	H	-	-	
				Pr	Ph1	-	C ₂ H ₅	H	-	-	-	-	-	-	
382	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	R6	R7	R8
				Pr	Ph1	-	-	H	-	-	-	-	-	-	-
383	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H	-	-
				Py1	Ph1	-	-	H	-	-	-	-	-	-	-
384	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OC ≡ C-C ₇ H ₁₅	H	H	-	-
				Py2	Ph1	-	-	H	-	-	-	-	-	-	-

Table 28 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1		CyN1-R2		CyN1			
								R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8
												CyC1			
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	R5	R6	R7	R8	CyN2	
								R"	R'''	CyC2-R3	CyC2-R4	R5	R6	R7	R8
385	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H		FL5	H	Ph3	H	-	
				Pi	Ph1	-	-	H	H	Ph2	H	H	H	H	
						-	-	CH ₃	CH ₃	-	-	-	-	-	
386	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H		FL5	H	Ph3	H	-	
				Pi	Ph1	-	-	H	H	Tn8	H	H	-	-	
						-	-	Br	Br	-	-	-	-	-	
387	Ir	1	2	Pi	Ph1	-	-	H	H	FL5	H	H	H	-	
				Pi	Ph1	CH ₃	CH ₃	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	
388	Ir	1	2	Pi	Ph1	-	-	H	CF ₃	H	-	-	-	-	
				Pi	Ph1	Ph3	Ph3	H	H	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	
						C ₅ H ₁₁	H	-	-						

Table 28 (continued)

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	
CyC1													
				R"	R'''	CyC1-R3	CyC1-R4			R5	R6	R7	R8
										R5	R6	R7	R8
CyN2													
				CyN2	Cyc2	R	R'	CyN2-R1	CyN2-R2				
						R"	R'''	Cyc2-R3	Cyc2-R4				
										R5	R6	R7	R8
CyC2													
										R5	R6	R7	R8
389	Ir	1	2	Pi	Np2	-	-	H	FL5	H	H	H	-
						Ph3	Ph3	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	OCH ₃	H	-	-	-	-
390	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	FL5	H	H
						CH ₃	CH ₃	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	Cl	H	-	-	-	-

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Table 29

No	M	m	n	CyN1	CyC1	R	R'	R"	R'''	CyN1-R1		CyN1-R2		CyN1	
										CyC1-R3	CyC1-R4	R5	R6	R7	R8
391	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-
				Pi	Tn1	-	-	H	H	-	-	-	-	-	-
392	Ir	1	2	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	R5	R6	R7	R8
				Pi	Tn1	-	-	H	H	-	-	-	-	-	-
393	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-
				Pi	Tn2	-	-	H	H	-	-	-	-	-	-
394	Ir	1	2	Pi	FL2	C ₄ H ₉	C ₄ H ₉	H	H	-	-	-	-	-	-
				Pi	Tn3	-	-	H	H	-	-	-	-	-	-

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Table 29 (continued)

No	M	m	n	C _y N1	C _y C1	R	R'	R''	C _y N1-R1		C _y N1-R2		C _y N1	
									C _y C1-R3	C _y C1-R4	R5	R6	R7	R8
				C _y N2	C _y C2	R	R'	R''	C _y N2-R1	C _y N2-R2	R5	R6	R7	R8
395	Ir	1	2	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇		H	H	-	-	-	-
				Pi	Tn4	-	-		H	H	-	-	-	-
396	Ir	1	2	Pi	FL2	H	H		H	H	-	-	-	-
				Pi	Np1	CH ₃	CH ₃		H	H	FL5	H	H	-
397	Ir	1	2	Pi	FL2	CH ₃	CH ₃		H	H	-	-	-	-
				Pi	Np2	CH ₃	CH ₃		H	H	FL5	H	H	-
398	Ir	1	2	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁		H	H	-	-	-	-
				Pi	Pe1	-	-		H	H	-	-	-	-
									H	H	-	-	-	-

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Table 29 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1					
										R5	R6	R7	R8		
				R"	CyC1-R3	CyC1-R4	Cyc1								
							R5				R6	R7	R8		
							CyN2	CyC2	R'	CyN2-R1	CyN2-R2	Cyn2			
							R"	R"	CyC2-R3	CyC2-R4	Cyc2				
											R5	R6	R7	R8	
399	Ir	1	2	Pi	Fl2	CH ₃	Ph3	H	Fl5	H	H	H	-		
				Pi		CH ₃	Ph3	H	H	-	-	-	-		
				Pi	Cn1	-	-	H	H	-	-	-	-		
				Pi		-	-	H	-	-	-	-	-		
400	Ir	1	2	Pi	Fl2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	Fl5	H	H	H	-		
				Pi	Cn2	-	-	H	H	-	-	-	-		
				Pi		-	-	H	-	-	-	-	-		

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Table 30

No	M	m	n	CyN1	Cyc1	R	R"	R'	CyN1-R1	CyN1-R2	CyN1		
											Cyc1		R5
											R6	R7	R8
401	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	DBT3	H	H	H	-
				Pi	FL1	-	-	H	-	-	-	-	-
402	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-	-
403	Ir	1	2	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	Tn5	H	H	-	-
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-	-
404	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	Np3	H	H	-	-
				Pi	FL2	CH ₃	CH ₃	H	-	-	-	-	-

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Table 30 (continued)

No	M	m	n	Cyn1	Cyc1	R	R'	R"	Cyn1-R1		Cyn1-R2		Cyn1	
									Cyc1-R3	Cyc1-R4	R5	R6	R7	R8
											R5	R6	R7	R8
				Cyn2	CyC2	R	R'	R"	Cyn2-R1	Cyn2-R2	Cyn2			
											R5	R6	R7	R8
									Cyc2-R3	Cyc2-R4	Cyc2			
											R5	R6	R7	R8
405	Ir	1	2	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	-	H	H	-	-	-	-
				Pi	FL2	(CH ₂) ₅ Ph ₃	(CH ₂) ₅ Ph ₃	-	H	H	-	-	-	-
406	Ir	1	2	Pi	FL2	Ph ₃	Ph ₃	-	H	H	-	-	-	-
				Pi	FL2	C ₃ H ₇	C ₃ H ₇	-	H	H	-	-	-	-
407	Ir	1	2	Pi	FL2	CH ₃	Ph ₃	-	H	H	-	-	-	-
				Pi	FL3	-	-	-	H	H	-	-	-	-
408	Ir	1	2	Pi	FL2	(CH ₂) ₅ Ph ₃	(CH ₂) ₅ Ph ₃	-	H	H	-	-	-	-
				Pi	DBF1	-	-	-	H	H	-	-	-	-

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Table 30 (continued)

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1		
										R5	R6	R7
						R"	R"	CyC1-R3	CyC1-R4	CyC1		
										R5	R6	R7
										R5	R6	R8
CyN2	Cyc2	R	R					CyN2-R1	CyN2-R2	CyN2		
										R5	R6	R7
										R5	R6	R8
						R"	R"	CyC2-R3	CyC2-R4	Cyc2		
										R5	R6	R7
										R5	R6	R8
409	Ir	1	2	Pi	FL2	H	H					
						CH ₃	CH ₃	H	H			
				Pi	DBT1	-	-	H	H			
410	Ir	1	2	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	-
						CH ₃	CH ₃	H				
				Pi	Qn1	-	-	H	H			

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Table 31

No	M	m	n	CyN1	CyC1	R	R'	R"	R'''	CyN1-R1		CyN1-R2		CyN1	
										CyC1-R3	CyC1-R4	R5	R6	R7	R8
411	Ir	1	2	Pi	Fl2	C ₂ H ₅	C ₂ H ₅			FL5	H	H	H	-	
						C ₂ H ₅	C ₂ H ₅				H	-	-	-	
				Pr	Qn2	-	-			H	H	-	-	-	
412	Ir	1	2	Pi	Fl2	CH ₃	CH ₃			Ph2	H	H	H	H	
				Pr	Cz	-	-			H	H	-	-	-	
										Ph3	H	-	-	-	
413	Rh	1	2	Pi	Fl2	CH ₃	CH ₃			Ph2	H	OCH ₂ C ₅ F ₁₁	H	H	
										H	-	-	-	-	
414	Rh	1	2	Pi	Fl2	CH ₃	CH ₃			Ph2	H	OC≡C-C ₇ H ₁₅	H	H	
					Py2	Ph1	-			H	H	-	-	-	
						-				H	H	-	-	-	

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Table 31 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1				
										R5	R6	R7	R8	
				R"	R'''	CyC1-R3	CyC1-R4			CyC1				
										R5	R6	R7	R8	
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2				
						R"	R'''	CyC2-R3	CyC2-R4		R5	R6	R7	R8
										CyC2				
415	Rh	1	2	Pi	FL2	CH ₃	H		FL5	H	Ph3	H	-	
						CH ₃	H		Ph2	H	H	H	H	
				Pi	Ph1	-	H			-	-	-	-	
						-	-	CH ₃	H	-	-	-	-	
416	Rh	1	2	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-	
						CH ₃	CH ₃	H	Tn8	H	H	-	-	
				Pi	Ph1	-	H	H	-	-	-	-	-	
						-	-	Br	H	-	-	-	-	
417	Rh	1	2	Pi	Ph1	-	H		FL5	H	H	H	-	
						CH ₃	CH ₃	H		-	-	-	-	
				Pi	Ph1	-	H			-	-	-	-	
						-	-	CF ₃	H	-	-	-	-	
418	Rh	1	2	Pi	Ph1	-	H		FL5	H	H	H	-	
						Ph3	H			-	-	-	-	
				Pi	Ph1	-	H	H		-	-	-	-	
						-	-	C ₅ H ₁₁	H	-	-	-	-	

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Table 31 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
				R"	R"	CyC1-R3	CyC1-R4						
										R5	R6	R7	R8
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2				
						R"	R"	CyC2-R3	CyC2-R4				
										R5	R6	R7	R8
419	Rh	1	2	Pi	Np2	-	-	H	FL5	H	H	H	-
				Pi	Ph1	-	-	H		-	-	-	-
						-	-	OCH ₃	H	-	-	-	-
420	Rh	1	2	Pi	FL2	CH ₃	CH ₃	Ph2	H	FL5	H	H	
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	Cl	H	-	-	-	-

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Table 32

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2			
						R"	R'''	CyC2-R3	CyC2-R4	CyC2			
										R5	R6	R7	R8
421	Pt	1	1	Pi	FL1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
422	Pt	1	1	Pi	FL1	-	-	H	FL4	H	H	H	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
423	Pt	1	1	Pi	FL1	-	-	H	Ph2	H	H	H	H
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
424	Pt	1	1	Pi	FL1	-	-	H	FL4	H	Ph3	H	-
						-	-	H	Ph2	H	H	H	H
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
425	Pt	1	1	Pi	FL1	-	-	H	Np4	H	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
426	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
427	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

Table 32 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
5						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
10				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2			
										R5	R6	R7	R8
15						R"	R'''	CyC2-R3	CyC2-R4	CyC2			
										R5	R6	R7	R8
428	Pt	1	1	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
429	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-
						-	-	H	OC ₄ H ₉	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
430	Pt	1	1	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

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Table 33

No	M	m	n	CyN1	CyC1	R	R"	R"	CyC1-R3	CyN1-R1	CyN1-R2	CyN1			
												R5	R6	R7	R8
431	Pt	1	1	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	FL5	H	H	H	-	-	-
						C ₂ H ₅	C ₂ H ₅	H		-	-	-	-	-	-
				Pr	Ph1	-	-	H		-	-	-	-	-	-
						-	-	H		-	-	-	-	-	-
432	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H	H	H	H
					Pr	Ph1	-	-	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
433	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H	H	H
					Py1	Ph1	-	-	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-
434	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OC≡C-C ₇ H ₁₅	H	H	H	H
					Py2	Ph1	-	-	H	-	-	-	-	-	-
						-	-	H	H	-	-	-	-	-	-

Table 33 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1		
										R5	R6	R7
				R"	R'''			CyC1-R3	CyC1-R4	R5	R6	R7
										R5	R6	R7
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	R5	R6	R7
										R5	R6	R7
						R"	R'''	CyC2-R3	CyC2-R4	R5	R6	R7
										R5	R6	R7
435	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H
						CH ₃	CH ₃	H	Ph2	H	H	H
				Pi	Ph1	-	-	H	H	-	-	-
						-	-	CH ₃	H	-	-	-
436	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-
						-	-	H	H	-	-	-
				Pi	Tn1	-	-	H	CF ₃	-	-	-
						-	-	H	H	-	-	-
437	Pt	1	1	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-
						-	-	H	H	-	-	-
				Pi	Tn1	-	-	H	H	-	-	-
						-	-	H	H	-	-	-
438	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	OC ₄ H ₉	-	-
						-	-	H	H	-	-	-
				Pi	Tn2	-	-	H	H	-	-	-
						-	-	H	H	-	-	-

Table 33 (continued)

Table 34

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1			CyN1-R2			CyN1		
								R"	R'''	CyC1-R3	CyC1-R4	R5	R6	R7	R8	
441	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	DBT3	H	H	H	-	-	
						-	-	H	H	-	-	-	-	-	-	
				Pi	FL1	-	-	H	H	-	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	
442	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	H	Ph2	H	H	H	H	H	
						-	-	H	H	-	-	-	-	-	-	
				Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	
443	Pt	1	1	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	Tn5	H	H	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	
				Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	
444	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Np3	H	H	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	
				Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-	-	-	
						-	-	H	H	-	-	-	-	-	-	

Table 34 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
				CyN2	CyC2	R	R'	CyN2-R1	CyN2-R2	CyN2			
										R5	R6	R7	R8
						R"	R'''	CyC2-R3	CyC2-R4	CyC2			
										R5	R6	R7	R8
445	Pt	1	1	Pi	FL2	C ₈ H ₁₇	C ₈ H ₁₇	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
446	Pt	1	1	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	FL5	H	H	H	-
						C ₂ H ₅	C ₂ H ₅	H	-	-	-	-	-
				Pi	Qn2	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
447	Pt	1	1	Pi	FL2	CH ₃	CH ₃	CH ₃	Ph2	H	H	H	H
						-	-	H	H	-	-	-	-
				Pi	Cz	-	-	H	H	-	-	-	-
						-	-	Ph3	H	-	-	-	-
448	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H
						-	-	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

Table 34 (continued)

Table 35

No	M	m	n	CyN1	CyC1	R	R'	R''	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
451	Pt	1	1	Pi	Ph1	-	-	H	-	FL4	H	H	H	-
				Pi	Ph1	-	-	H	H	-	-	-	-	-
452	Pt	1	1	Pi	Np2	-	-	H	-	FL4	H	H	H	-
				Pi	Ph1	-	-	H	H	-	-	-	-	-
453	Pt	1	1	Pi	FL1	-	-	H	-	Ph2	H	FL4	H	H
				Pi	Ph1	-	-	H	H	-	-	-	-	-
454	Pt	1	1	Pi	Ph1	-	-	H	H	-	-	-	-	-
				Pi	Ph1	-	-	FL4	H	H	H	H	-	-
						-	-	H	H	-	-	-	-	-

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Table 35 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	Cyn1			
										R5	R6	R7	R8
Cyn2													
							R"	CyC1-R3	CyC1-R4	Cyc1			
										R5	R6	R7	R8
Cyn2													
							R'	CyN2-R1	CyN2-R2	Cyn2			
							R"	CyC2-R3	CyC2-R4	Cyc2			
										R5	R6	R7	R8
455	Pt	1	1	Pi	Ph1	-	-	H	Ph2	H	FL4	H	H
				Pi	Ph1	-	-	H	H	-	-	-	-
456	Pt	1	1	Pi	Fl2	Ph3	Ph3	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
457	Pt	1	1	Pi	Fl2	CH ₃	Ph3	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
458	Pt	1	1	Pi	Fl2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	H	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
								H	H	-	-	-	-

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Table 35 (continued)

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Table 36

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
				R"	CyC1-R3	CyC1-R4				R5	R6	R7	R8
										R5	R6	R7	R8
										R5	R6	R7	R8
461	Pt	1	1	Pi	Fl2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-
						CH ₃	CH ₃	H	Tn8	H	H	-	-
				Pi	Ph1	-	-	H	-	-	-	-	-
						-	-	Br	H	-	-	-	-
462	Pt	1	1	Pi	Ph1	-	-	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	-	-	-	-	-
				Pi	Ph1	-	-	H	-	-	-	-	-
						-	-	CF ₃	H	-	-	-	-
463	Pt	1	1	Pi	Ph1	-	-	H	FL5	H	H	H	-
						Ph3	Ph3	H	-	-	-	-	-
				Pi	Ph1	-	-	H	-	-	-	-	-
						-	-	C ₅ H ₁₁	H	-	-	-	-
464	Pt	1	1	Pi	Np2	-	-	H	FL5	H	H	H	-
						Ph3	Ph3	H	-	-	-	-	-
				Pi	Ph1	-	-	H	H	-	-	-	-
						-	-	OCH ₃	H	-	-	-	-

Table 36 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1				
										R5	R6	R7	R8	
CyC1-R4														
465	Pt	1	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	FL5	H	H	
				Pi	Ph1	-	-	H	H	-	-	-	-	
				Pd	1	1	FL2	H	H	FL5	H	H	H	
				Pi	Np1	CH ₃	CH ₃	H	H	-	-	-	-	
				Pd	1	1	Pi	FL2	CH ₃	CH ₃	H	H	H	-
				Pi	Np2	CH ₃	CH ₃	H	H	-	-	-	-	
				Pd	1	1	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	FL5	H	H	-
									C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	-	-	-
									Pi	Pe1	-	H	-	-
										-	H	H	-	-

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Table 36 (continued)

No	M	m	n	C _y N1	C _y C1	R	R'	C _y N1-R1	C _y N1-R2	C _y N1			
										R5	R6	R7	R8
						R"	R'''	C _y C1-R3	C _y C1-R4	C _y C1			
										R5	R6	R7	R8
				C _y N2	C _y C2	R	R'	C _y N2-R1	C _y N2-R2	C _y N2			
										R5	R6	R7	R8
						R"	R'''	C _y C2-R3	C _y C2-R4	C _y C2			
										R5	R6	R7	R8
469	Pd	1	1	Pi	FL2	CH ₃	Ph3	H	FL5	H	H	H	-
						CH ₃	Ph3	H		-	-	-	-
				Pi	Cn1	-	-	H		-	-	-	-
						-	-	H		-	-	-	-
470	Pd	1	1	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	FL5	H	H	H	-
						CH ₃	CH ₃	H		-	-	-	-
				Pi	Cn2	-	-	H		-	-	-	-
						-	-	H		-	-	-	-

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Table 37

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
						R"	R'''	CyC1-R3	CyC1-R4	CyC1			
										R5	R6	R7	R8
								CyN2-R1	CyN2-R2	CyN2			
										R5	R6	R7	R8
						R"	R'''	CyC2-R3	CyC2-R4	CyC2			
										R5	R6	R7	R8
471	Pd	1	1	Pi	FL2	Ph3	Ph3	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
472	Pd	1	1	Pi	FL2	CH ₃	Ph3	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	FL3	-	-	H	H	-	-	-	-
								H	H	-	-	-	-
473	Pd	1	1	Pi	FL2	(CH ₂) ₅ Rh3	(CH ₂) ₅ Ph3	H	H	-	-	-	-
						-	-	H	H	-	-	-	-
				Pi	DBF1	-	-	H	H	-	-	-	-
								H	H	-	-	-	-
474	Pd	1	1	Pi	FL2	H	H	H	FL5	H	H	H	-
						CH ₃	CH ₃	H	H	-	-	-	-
				Pi	DBT1	-	-	H	H	-	-	-	-
						-	-	H	H	-	-	-	-

Table 37 (continued)

Table 37 (continued)

Table 38

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1												
										R5	R6	R7	R8									
CyC1																						
CyC1																						
481	Ir	3	0	Pi	FL1	-	-	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
482	Ir	3	0	Pi	FL1	-	-	H	CF ₃	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
483	Ir	3	0	Pi	FL1	-	-	H	FL4	H	H	H	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
484	Ir	3	0	Pi	FL1	-	-	H	Ph2	H	H	H	H									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
485	Ir	3	0	Pi	FL1	-	-	H	FL4	H	Ph3	H	-									
						-	-	-CH=CH-CH=CH-		H	H	H	H									
486	Ir	3	0	Pi	FL1	-	-	H	Np4	H	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
487	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
488	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
489	Ir	3	0	Pi	FL2	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
490	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	CH ₃	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
491	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
492	Ir	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
493	Ir	3	0	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
494	Ir	3	0	Pi	FL2	C ₄ H ₉	C ₄ H ₉	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
495	Ir	3	0	Pi	FL2	Ph3	Ph3	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
496	Ir	3	0	Pi	FL2	CH ₃	Ph3	H	H	-	-	-	-									
						-	-	-CH=CH-CH=CH-		-	-	-	-									
497	Ir	3	0	Pi	FL2	H	H	H	FL5	H	H	H	-									
						CH ₃	CH ₃	-CH=CH-CH=CH-		-	-	-	-									

Table 38 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
CyC1													
5						R"	R'''	CyC1-R3	CyC1-R4				
10	498	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	H
15							CH ₃	CH ₃	-CH=CH-CH=CH-		-	-	-
20	499	Ir	3	0	Pi	FL2	C ₂ H ₅	C ₂ H ₅	H	FL5	H	H	H
25							C ₂ H ₅	C ₂ H ₅	-CH=CH-CH=CH-		-	-	-
30	500	Ir	3	0	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	FL5	H	H	H
35							C ₅ H ₁₁	C ₅ H ₁₁	-CH=CH-CH=CH-		-	-	-
40	501	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	H
45							C ₈ H ₁₇	C ₈ H ₁₇	-CH=CH-CH=CH-		-	-	-
50	502	Ir	3	0	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	H	H
55							-	-	-CH=CH-CH=CH-		-	-	-

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Table 39

No	M	m	n	CyN1	Cyc1	R	R'	CyN1-R1	CyN1-R2	CyN1			
										R5	R6	R7	R8
503	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Ph2	C ₆ F ₅	H	H	H
504	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Ph2	H	OCH ₂ C ₅ F ₁₁	H	H
505	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Ph2	H	OC≡C-C ₇ H ₁₅	H	H
506	Ir	3	0	Pi	Fl2	C ₃ H ₇	C ₃ H ₇	H	-	-	-	-	-
507	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Tn5	H	H	-	-
508	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Np3	H	H	-	-
509	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Np4	H	-	-	-
510	Ir	3	0	Pi	Fl2	CH ₃	CH ₃	H	Tn7	H	H	-	-

Table 40

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1					
										R5	R6	R7	R8		
						R"	R'''	CyC1-R3	CyC1-R4	CyC1					
										R5	R6	R7	R8		
				E		R"	R'''			E					
										R5	R6	R7	R8		
				G		R"	R'''			G					
										R5	R6	R7	R8		
511	Ir	2	1	Pi	FL1	-	-	H	H	-	-	-	-		
						-	-	H	H	-	-	-	-		
				CH ₃		-	-			-	-	-	-		
				CH ₃		-	-			-	-	-	-		
				Pi	FL1	-	-	H	CF ₃	-	-	-	-		
512	Ir	2	1			-	-	H	H	-	-	-	-		
						-	-	H	H	-	-	-	-		
			CF ₃			-	-			-	-	-	-		
			CF ₃			-	-			-	-	-	-		
			Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-			
513	Ir	2			1			-	-	H	H	-	-	-	-
			CH ₃		-	-			-	-	-	-			
			CH ₃		-	-			-	-	-	-			
			Pi	FL2	CH ₃	CH ₃	H	CF ₃	-	-	-	-			
					-	-	H	H	-	-	-	-			
514	Ir	2	1		Ph2		-	-			H	H	H	H	
					Ph2		-	-			H	H	H	H	
					Ph2		-	-			H	C ₃ H ₇	H	H	
					Ph2		-	-			H	C ₃ H ₇	H	H	
				Pi	FL2	CH ₃	CH ₃	H	H	-	-	-	-		
515	Ir	2	1			-	-	H	OC ₄ H ₉	-	-	-	-		
			Ph2			-	-			H	C ₃ H ₇	H	H		
			Ph2			-	-			H	C ₃ H ₇	H	H		
			Pi	FL2	C ₆ H ₁₃	C ₆ H ₁₃	H	H	-	-	-	-			
					-	-	H	H	-	-	-	-			
516	Ir	2	1		CH ₃		-	-			H	H	-	-	
					FL5		CH ₃	CH ₃			H	H	H	-	
				Pi	FL2	H	H	H	FL5	H	H	H	-		
						CH ₃	CH ₃	H	H	-	-	-	-		
				Tn5		-	-			H	H	-	-		
517	Ir	2	1	Tn5		-	-			H	H	-	-		
				Tn5		-	-			H	H	-	-		
										H	H	-	-		

Table 40 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1					
										R5	R6	R7	R8		
5						R"	R'''	CyC1-R3	CyC1-R4	CyC1					
										R5	R6	R7	R8		
				E		R"	R'''			E					
10										R5	R6	R7	R8		
				G		R"	R'''			G					
										R5	R6	R7	R8		
15	518	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	H	H	-	
							CH ₃	CH ₃	H	H	-	-	-	-	
					Tn6		-	-			H	H	-	-	
					Tn6		-	-			H	H	-	-	
20	519	Ir	2	1	Pi	FL2	Ph3	Ph3	H	FL5	H	H	H	-	
							Ph3	Ph3	H	H	-	-	-	-	
					CH ₃		-	-			-	-	-	-	
					CH ₃		-	-			-	-	-	-	
25	520	Ir	2	1	Pi	FL2	CH ₃	Ph3	H	FL5	H	H	H	-	
							CH ₃	Ph3	H	H	-	-	-	-	
					CF ₃		-	-			-	-	-	-	
					CF ₃		-	-			-	-	-	-	

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Table 41

No	M	m	n	CyN1	CyC1	R	R'	R"	R'''	CyN1-R1		CyN1-R2		CyN1	
										CyC1-R3	CyC1-R4	R5	R6	R7	R8
												R5	R6	R7	R8
												E	E	E	E
												G	G	G	G
												R5	R6	R7	R8
521	Ir	2	1	Pi	FL2	(CH ₂) ₅ Ph3	(CH ₂) ₅ Ph3	H	FL5	H	H	H	H	-	-
						CH ₃	CH ₃	H	H	-	-	-	-	-	-
				Np3	-	-	-			CH ₃ O	H	-	-	-	-
				Np3	-	-	-			CH ₃ O	H	-	-	-	-
522	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Pr2	H	H	H	H	H	H
						-	-	H	H	-	-	-	-	-	-
				Np4	-	-	-			F	-	-	-	-	-
				Np4	-	-	-			F	-	-	-	-	-
523	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Pr2	H	OCH ₂ C ₅ F ₁₁	H	H	H	H
						-	-	H	H	-	-	-	-	-	-
				Tn7	-	-	-			CH ₃	-	-	-	-	-
				Tn7	-	-	-			CH ₃	-	-	-	-	-
524	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Pr2	H	OC≡C-C ₇ H ₁₅	H	H	H	H
						-	-	H	H	-	-	-	-	-	-
				Tn8	-	-	-			H	-	-	-	-	-
				Tn8	-	-	-			H	-	-	-	-	-

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Table 41 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
525	Ir	2	1	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	Tn5	H	H	-	-	-
				Pe2	-	-	-	H	H	-	-	-	-	-
				Pe2	-	-	-	-	-	H	-	-	-	-
526	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL4	H	Ph3	H	-	-
				Pi2	-	-	-	H	Ph2	H	H	H	-	-
				Pi2	-	-	-	-	-	H	H	-	-	-
527	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	FL5	H	Ph3	H	-	-
				Pi3	-	-	-	-	-	CH ₃	CH ₃	H	H	-
				Pi3	-	-	-	-	-	CH ₃	CH ₃	H	H	-
528	Ir	2	1	Pi	Ph1	CH ₃	CH ₃	H	FL5	H	H	H	H	-
				FL4	-	-	-	-	-	H	H	H	H	-
				FL4	-	-	-	-	-	H	H	H	H	-

Table 41 (continued)

No	M	m	n	CyN1	CyC1	R	R'	R"	CyN1-R1		CyN1-R2		CyN1	
									CyC1-R3	CyC1-R4	R5	R6	R7	R8
						R"	R"	R"			R5	R6	R7	R8
				E		R"	R"							
				G		R"	R"							
529	Ir	2	1	Pi	FL2	CH ₃	CH ₃	H	Ph2	H	R5	R6	R7	R8
						CH ₃	CH ₃	H	H	-				
				FL5	C ₂ H ₅									
				FL5	(CH ₂) ₅ Ph3									
530	Ir	2	1	Pi	Ph1	-	-	H	H	-	-	-	-	-
						C ₈ H ₁₇		C ₈ H ₁₇	FL5	H	H	H	H	-
				DBF2	-						H	H	H	-
				DBF2	-						H	H	H	-

Table 42

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1				
										R5	R6	R7	R8	
5						R"	R'''	CyC1-R3	CyC1-R4	CyC1				
										R5	R6	R7	R8	
10						E	R"	R'''			E			
										R5	R6	R7	R8	
15						G	R"	R'''			G			
										R5	R6	R7	R8	
531	Ir	2	1	Pi	Ph1	-	-	H	Ph2	H	FL5	H	H	
						CH ₃	CH ₃	H	H	-	-	-	-	
				DBT3		-	-			H	H	H	-	
				DBT3		-	-			H	H	H	-	
532	Rh	2	1	Pi	FL3	CH ₃	CH ₃	H	H	-	-	-	-	
						-	-	H	H	-	-	-	-	
				CH ₃		-	-			-	-	-	-	
				CH ₃		-	-			-	-	-	-	
533	Rh	2	1	Pi	DBF1	CH ₃	CH ₃	CF ₃	CF ₃	-	-	-	-	
						-	-	H	H	-	-	-	-	
				CF ₃		-	-			-	-	-	-	
				CF ₃		-	-			-	-	-	-	
534	Rh	2	1	Pi	FL1	-	-	H	FL5	H	H	H	-	
						CH ₃	CH ₃	H	H	-	-	-	-	
				Qn2		-	-			H	H	-	-	
				Qn2		-	-			H	H	-	-	
535	Rh	2	1	Pi	Np2	-	-	H	FL4	H	H	H	-	
						-	-	H	H	-	-	-	-	
				Np3		-	-			H	H	-	-	
				Np3		-	-			H	H	-	-	
536	Pt	1	1	Pi	FL2	C ₃ H ₇	C ₃ H ₇	H	H	-	-	-	-	
						-	-	H	H	-	-	-	-	
				CH ₃		-	-			-	-	-	-	
				CH ₃		-	-			-	-	-	-	
537	Pt	1	1	Pi	FL2	C ₅ H ₁₁	C ₅ H ₁₁	H	H	-	-	-	-	
						-	-	H	H	-	-	-	-	
				CF ₃		-	-			-	-	-	-	
				CF ₃		-	-			-	-	-	-	

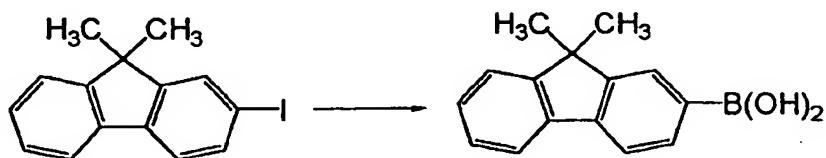
Table 42 (continued)

No	M	m	n	CyN1	CyC1	R	R'	CyN1-R1	CyN1-R2	CyN1					
										R5	R6	R7	R8		
5						R"	R'''	CyC1-R3	CyC1-R4	CyC1					
										R5	R6	R7	R8		
				E		R"	R'''			E					
10										R5	R6	R7	R8		
				G		R"	R'''			G					
										R5	R6	R7	R8		
15	538	Pd	1	1	Pi	FL2	C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	FL5	H	H	H	-	
							C ₁₅ H ₃₁	C ₁₅ H ₃₁	H	H	-	-	-	-	
					CH ₃		-	-			-	-	-	-	
					CH ₃		-	-			-	-	-	-	
20	539	Pd	1	1	Pi	FL2	CH ₃	CH ₃	H	Np3	H	H	-	-	
							-	-	H	H	-	-	-	-	
					CF ₃		-	-			-	-	-	-	
					CF ₃		-	-			-	-	-	-	
25	540	Ir	1	2	Pi	Tn4	-	-	H	FL5	H	H	H	-	
							CH ₃	CH ₃	H	H	-	-	-	-	
					CH ₃		-	-			-	-	-	-	
30					CH ₃		-	-			-	-	-	-	

[0063] Hereinbelow, the present invention will be described more specifically based on Examples.

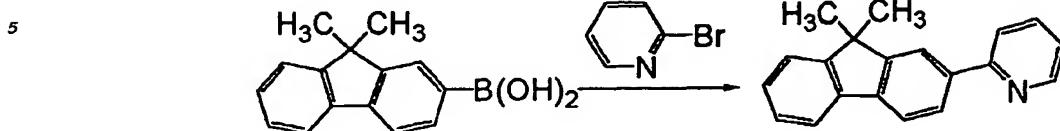
Example 1 (Synthesis of Example Compound No. 23)

[0064]

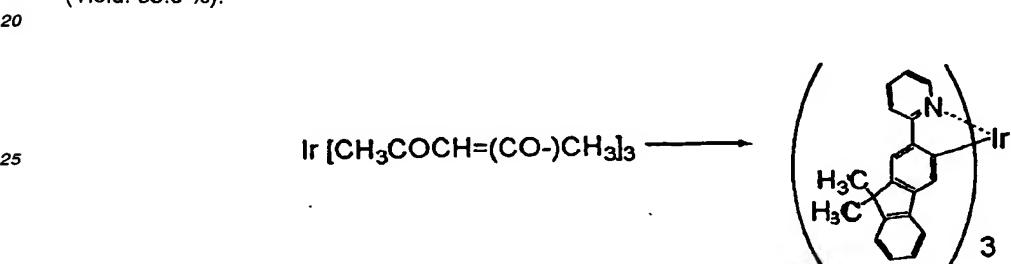


[0065] In a 30 liter-three-necked flask, 307.3 g (960 mM) of 2-iodo-9,9-dimethylfluorene and 10 liters of dry THF (tetrahydrofuran) were placed and cooled to -72 to 70 °C under stirring in an argon gas stream atmosphere. To the mixture, a 1.6M solution of n-butyllithium in hexane was added dropwise in 1 hour, followed by further stirring for 2 hours at the temperature. Thereafter, under stirring at -73 to -71 °C, to the system, a solution of 209.5 g (2016 mM) of trimethyl borate in 1.3 liters of dry THT was added dropwise in 2 hours. The reaction mixture was left standing overnight on an ice water bath. To the mixture, 1.6 liters of 4N-hydrochloric acid was added in 0.5 hour at 0 - 7 °C, followed by stirring for 1 hour at room temperature and extraction with toluene. The organic layer was washed with saturated saline water, followed by distilling-off of the solvent under a reduced pressure to obtain a residue. To the residue, hexane was added and heated under heating, followed by cooling to precipitate a crystal. The crystal was recovered by filtration and purified by silica gel column chromatography (eluent: toluene/ethyl acetate = 1/1), followed by successive recrystallization from a chloroform-hexane mixture solvent, toluene, an ethyl acetate-toluene-THF mixture solvent, and tol-

uene to obtain 32.0 g of 2-(9,9-dimethylfluorenyl)boronic acid (colorless crystal) (Yield: 14.0 %).



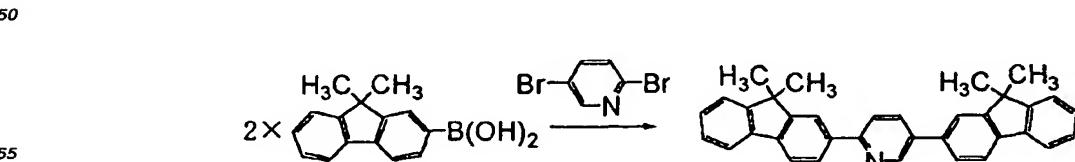
10 [0066] In a 300 ml-three-necked flask, 8.5 g (53.8 mM) of 2-bromopyridine, 12.8 g (53.8 mM) of 2-(9,9-dimethylfluorenyl)boronic acid, 55 ml of toluene, 27 ml of ethanol and 55 ml of 2M-sodium carbonate aqueous solution were placed and stirred at room temperature under nitrogen stream, and 1.97 g (1.70 mM) of tetrakis(triphenylphosphine) palladium (0) was added thereto. Thereafter, reflux under stirring for 5.5 hours was performed under nitrogen stream.
15 After the reaction, the reaction mixture was cooled and extracted by addition of cold water and toluene. The organic layer was washed with water until neutrality, and the solvent was removed under reduced pressure to obtain a residue. The residue was successively purified by silica gel column chromatography (eluent: toluene/THF = 10/1) and that (eluent: hexane/ethyl acetate = 8/1) to obtain 12.2 g of 2-[2-(9,9-dimethylfluorenyl)]pyridine (pale brown viscous liquid) (Yield: 83.6 %).
20



30 [0067] In a 100 ml-four-necked flask, 50 ml of glycerol was placed and heated at 130 - 140 °C under stirring and bubbling with nitrogen for 2 hours. Then, the glycerol was cooled by standing down to 100 °C, and 1.69 g (6.23 mM) of 2-[2-(9,9-dimethylfluorenyl)]pyridine and 0.50 g (1.02 mM) of iridium (III) acetylacetonate were added, followed by 5 hours of heating at 176 - 219 °C under stirring and nitrogen stream. The reaction product was cooled to room temperature and injected into 300 ml of 1N-hydrochloric acid to form a precipitate, which was filtered out and washed with water, followed by drying for 5 hours at 100 °C under reduced pressure. The precipitate was purified by silica gel column chromatography with chloroform as the eluent to obtain 0.17 g (yield = 21.3 %) of orange powdery tris[2-(9,9-dimethylfluorene-2-yl)pyridine-C³,N]iridium (III). According to MALDI-TOF MS (matrix-assisted laser desorption ionization-time of flight mass spectroscopy), the compound exhibited M⁺ (mass number of the corresponding cation formed by removal of 1 electron) of 1003.4.
35 [0068] A toluene solution of the compound exhibited a photoluminescence spectrum showing λ_{max} (maximum emission wavelength) = 545 nm and a quantum yield of 0.23.
40 [0069] The compound (Ex. Comp. No. 23) exhibited better synthesis yield and quantum yield, thus being most suitable luminescence material in the present invention.
45

Example 2 (Synthesis of Example Compound No. 43)

[0070]



55 [0071] In a 100 ml-three-necked flask, 1.18 g (4.98 mM) of 2,5-dibromopyridine, 3.57 g (15.0 mM) 2-(9,9-dimethyl-

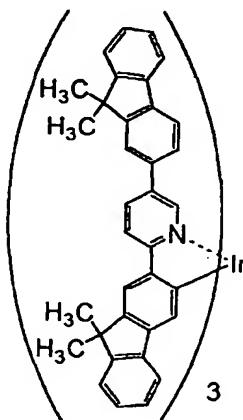
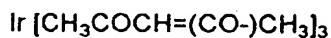
fluorenyl)boronic acid prepared in Example 1, 10 ml of toluene, 5 ml of ethanol and 10 ml of 2M-sodium carbonate aqueous solution were placed and stirred at room temperature under nitrogen stream, and 0.35 g (0.30 mM) of tetrakis (triphenylphosphine)-palladium (0) was added thereto. Thereafter, reflux under stirring was performed for 12 hours under nitrogen stream. After completion of the reaction, the reaction product was cooled on an ice bath to precipitate a crystal, which was then filtered out and washed with water. To the crystal, 100 ml of methanol was added and washed at room temperature under stirring, and then was recovered by filtration. The resultant crystal was purified by silica gel column chromatography (eluent: chloroform) to obtain 2.10 g (yield = 91.0 %) of 2,5-bis{2-(9,9-dimethylfluorenyl)}pyridine (colorless crystal).

10

15

20

25



[0072] In a 100 ml-four-necked flask, 50 ml of glycerol was placed and heated at 130 - 140 °C under stirring and bubbling with nitrogen for 2 hours. Then, the glycerol was cooled by standing down to 100 °C, and 1.85 g (3.99 mM) of 2,5-bis{2-(9,9-dimethylfluorenyl)}pyridine and 0.40 g (0.82 mM) of iridium (III) acetylacetone were added, followed by 5 hours of reflux at 180 - 235 °C under stirring and nitrogen stream. The reaction product was cooled to room temperature and injected into 300 ml of 1N-hydrochloric acid to form a precipitate, which was filtered out and washed with water, followed by drying for 5 hours at 100 °C under reduced pressure. The precipitate was purified by silica gel column chromatography with chloroform as the eluent and recrystallized from a chloroform-methanol mixture solvent to obtain 0.10 g (yield = 7.7 %) of red powdery tris[2,5-bis(9,9-dimethylfluorene-2-yl)pyridine-C³,N]iridium (III). According to MALDI-TOF MS, the compound exhibited M⁺ of 1589.6.

[0073] A toluene solution of the compound exhibited a photoluminescence spectrum showing $\lambda_{\text{max}} = 591 \text{ nm}$ and a quantum yield of 0.12.

40 Examples 3 - 11

[0074] Each of luminescence devices having a layer structure shown in Figure 1B were prepared in the following manner.

[0075] On a 1.1 mm-thick glass substrate (transparent substrate 15), a 100 nm-thick film (transparent electrode 14) of ITO (indium tin oxide) was formed by sputtering, followed by patterning to form a stripe electrode including 100 lines each having a width of 100 nm and a spacing with an adjacent line of 10 nm (i.e., electrode pitch of 110 nm).

[0076] On the ITO-formed substrate, three organic layers and two metal electrode layers shown below were successively formed by vacuum (vapor) deposition using resistance heating in a vacuum chamber (10⁻⁴ Pa).

Organic layer 1 (hole transport layer 13) (40 nm): α -NPD

Organic layer 2 (luminescence layer 12) (30 nm): co-deposited film of CBP:metal complex (metal coordination compound shown in Table 45) (95:5 by weight)

Organic layer 3 (electron transport layer 16) (30 nm): Alq₃

Metal electrode layer 1 (metal electrode 11) (15 nm): Al-Li alloy (Li = 1.8 wt. %)

Metal electrode layer 2 (metal electrode 11) (100 nm): Al

[0077] The above-deposited metal electrode layers 1 and 2 (Al-Li layer and Al layer) had a stripe electrode pattern including 100 lines each having a width of 100 nm and a spacing of 10 nm (electrode pitch = 110 nm) and arranged so that the stripe electrode pattern intersected with that of the ITO electrode at right angles to form a matrix of pixels each having an effective electrode area of 3 mm² comprising 20 ITO lines bundled together at a lead-out portion and

15 Al (Al-Li) lines bundled together at a lead-out portion.

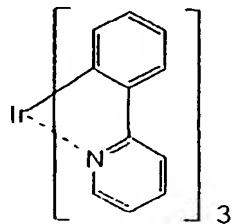
[0078] Each of the thus-prepared luminescence devices was taken out of the vacuum chamber and was subjected to a continuous energization (current passage) test in an atmosphere of dry nitrogen gas stream so as to remove device deterioration factors, such as oxygen and moisture (water content).

5 [0079] The continuous energization test was performed by continuously applying a voltage at a constant current density of 70 mA/cm² to the luminescence device having the ITO (transparent) electrode (as an anode) and the Al (metal) electrode (as a cathode), followed by measurement of emission luminance (brightness) with time so as to determine a time (luminance half-life) required for decreasing an initial luminance (60 - 220 cd/m²) to 1/2 thereof.

10 [0080] The results are shown in Table 45 appearing hereinafter.

Comparative Example 1

15 [0081] A comparative luminescence device was prepared and evaluated in the same manner as in Examples 3 - 11 except that the Ir complexes (metal coordination compounds shown in Table 45) was changed to Ir-phenylpyrimidine complex (Ir(ppy)₃) shown below.



[0082] The results are also also shown in Table 45 below.

30 Table 45

Ex. No.	Compound No.	Luminance half-life (Hr)
Ex. 3	6	700
Ex. 4	23	850
Ex. 5	43	950
Ex. 6	54	800
Ex. 7	72	850
Ex. 8	99	750
Ex. 9	118	600
Ex. 10	153	700
Ex. 11	440	650
Comp.Ex. 1	Ir(ppy) ₃	350

45 [0083] As is apparent from Table 45, compared with the conventional luminescence device using Ir(ppy)₃, the luminescence devices using the metal coordination compounds of formula (1) according to the present invention provide longer luminance half-lives, thus resulting in an EL device having a high durability (luminance stability) based on a good stability of the metal coordination compound of formula (1) of the present invention.

50 Example 12

[0084] A color organic EL display apparatus shown in Figure 2 was prepared in the following manner.

[0085] An active matrix substrate had a planar structure basically similar to a structure described in U.S. Patent No. 6,114,715.

55 [0086] Specifically, on a 1.1 mm-thick glass substrate, top gate-type TFTs of polycrystalline silicon were formed in an ordinary manner and thereon, a flattening film was formed with contact holes for electrical connection with a pixel electrode (anode) at respective source regions, thus preparing an active matrix substrate with a TFT circuit.

[0087] On the active matrix substrate, a 700 nm-thick pixel electrode (anode) of ITO having a large work function

was formed in a prescribed pattern. On the ITO electrode, prescribed organic layers and a 100 nm-thick Al electrode (cathode) were successively formed by vacuum deposition with a hard mask, followed by patterning to form a matrix of color pixels (128x128 pixels).

5 [0088] The respective organic layers corresponding to three color pixels (red (R) green (G) and blue (B)) were consisting of the following layers.

<R pixel region>

10 [0089]

α -NPD (40 nm)/CBP: Ex. Comp. No. 487 (93:7 by weight) (30 nm)/BCP (20 nm)/Alq 3 (40 nm)

<G pixel region>

15 [0090]

α -NPD (50 nm)/Alq 3 (50 nm)

<B pixel region>

20 [0091]

α -NPD (50 nm)/BCP (20 nm)/Alq 3 (50 nm)

25 [0092] When the thus-prepared color organic EL display apparatus was driven, desired color image data can be displayed stably with good image qualities.

Example 13 (Synthesis of Ex. Comp. No. 24)

30 [0093] It is easy to synthesize the following compound in the same manner as in Example 1 except for using 2-chloro-5-trifluoromethylpyridine (made by Tokyo Kasei Kogyo K.K.) instead of 2-bromopyridine in Example 1.

[0094] Tris[2-(9,9-dimethylfluorene-2-yl)-5-trifluoromethylpyridine-C³,N]iridium (III).

Example 14 (Synthesis of Ex. Comp. No. 25)

35 [0095] It is easy to synthesize the following compound in the same manner as in Example 1 except for using 2-chloro-4,5-bis(trifluoromethyl)pyridine (made by Oakwood Products Inc.) instead of 2-bromopyridine in Example 1.

[0096] Tris[2-(9,9-dimethylfluorene-2-yl)-4,5-bis(trifluoromethyl)pyridine-C³,N]iridium (III).

40 Example 15 (Synthesis of Ex. Comp. No. 26)

[0097] It is easy to synthesize the following compound in the same manner as in Example 1 except for using 2-chloro-5-methylpyridine (made by Aldrich Co.) instead of 2-bromopyridine in Example 1.

[0098] Tris[2-(9,9-dimethylfluorene-2-yl)-5-methylpyridine-C³,N]iridium (III).

45

Example 16 (Synthesis of Ex. Comp. No. 28)

50 [0099] It is easy to synthesize the following compound in the same manner as in Example 1 except that 2-bromo-9,9-diethylfluorene was synthesized from 2-bromofluorene and iodoethane in the same manner as the process described in Example 1 at page 32 of Japanese Laid-Open Patent Application (Tokuhyo Hei) 11-510535 (corr. to U.S. Patent No. 5,708,130) and was modified into 2-(9,9-diethylfluorenyl)borate in the same manner as in Example 1 (of the present application), followed by reaction with 2-bromopyridine to synthesize 2-{2-(9,9-diethylfluorenyl)pyridine and then reaction with iridium (III) acetylacetone in the same manner as in Example 1.

[0100] Tris[2-(9,9-diethylfluorene-2-yl)pyridine-C³,N]iridium (III).

55

Example 17 (Synthesis of Ex. Comp. No. 29)

[0101] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-io-

dopropane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0102] Tris{2-[9,9-di(1-propyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 18 (Synthesis of Ex. Comp. No. 30)

[0103] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iodobutane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0104] Tris{2-[9,9-di(1-butyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 19 (Synthesis of Ex. Comp. No. 31)

[0105] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iododopentane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0106] Tris{2-[9,9-di(1-pentyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 20 (Synthesis of Ex. Comp. No. 32)

[0107] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iodohexane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0108] Tris{2-[9,9-di(1-hexyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 21 (Synthesis of Ex. Comp. No. 33)

[0109] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iodoheptane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0110] Tris{2-[9,9-di(1-heptyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 22 (Synthesis of Ex. Comp. No. 34)

[0111] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iodooctane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0112] Tris{2-[9,9-di(1-octyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 23 (Synthesis of Ex. Comp. No. 35)

[0113] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-iodododecane (made by Aldrich Co.) instead of iodoethane and using 2-chloro-5-trifluoromethylpyridine (made by Tokyo Kasei Kogyo K.K.) instead of 2-bromopyridine, in Example 16.
[0114] Tris{2-[9,9-di(1-decyl)fluorene-2-yl]-5-trifluoromethylpyridine-C³,N}iridium (III).

Example 24 (Synthesis of Ex. Comp. No. 37)

[0115] It is easy to synthesize the following compound in the same manner as in Example 16 except for using 1-bromoecosane (made by Aldrich Co.) instead of iodoethane in Example 16.
[0116] Tris{2-[9,9-di(1-eicosyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 25 (Synthesis of Ex. Comp. No. 44)

[0117] It is easy to synthesize the following compound in the same manner as in Example 2 except for using 2-(9,9-diethylfluorenyl)boronic acid instead of 2-(9,9-dimethylfluorenyl)boronic acid in Example 2.
[0118] Tris[2,5-bis(9,9-diethylfluorene-2-yl)pyridine-C³,N]iridium (III).

Example 26 (Synthesis of Ex. Comp. No. 45)

[0119] It is easy to synthesize the following compound in the same manner as in Example 2 except for using 2-[9,9-di(1-pentyl)fluorenyl]boronic acid instead of 2-(9,9-dimethylfluorenyl)boronic acid in Example 2.
[0120] Tris{2,5-bis[9,9-di(1-pentyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 27 (Synthesis of Ex. Comp. No. 47)

[0121] It is easy to synthesize the following compound in the same manner as in Example 2 except for using 2-[9,9-di(1-pentadecyl)fluorenyl]boronic acid instead of 2-(9,9-dimethylfluorenyl)boronic acid in Example 2.

5 [0122] Tris{2,5-bis[9,9-di(1-pentadecyl)fluorene-2-yl]pyridine-C³,N}iridium (III).

Example 28 (Synthesis of Ex. Comp. No. 146)

10 [0123] It is easy to synthesize the following compound in the same manner as in Example 1 except for using dibenzofuran-4-boronic acid (made by Frontier Scientific Inc.) instead of 2-(9,9-dimethylfluorenyl)-boronic acid in Example 1.

[0124] Tris[2-(dibenzofuran)-4-yl]pyridine-C³,N]iridium (III).

Example 29 (Synthesis of Ex. Comp. No. 147)

15 [0125] It is easy to synthesize the following compound in the same manner as in Example 1 except for using dibenzothiophene-4-boronic acid (made by Frontier Scientific Inc.) instead of 2-(9,9-dimethylfluorenyl)boronic acid in Example 1.

[0126] Tris[2-(benzothiophene)-4-yl]pyridine-C³,N]iridium (III).

20 Example 30 (Synthesis of Ex. Comp. No. 149)

[0127] It is easy to synthesize the following compound in the same manner as in Example 2 except for using dibenzofuran-4-boronic acid (made by Frontier Scientific Inc.) instead of 2-(9,9-dimethylfluorenyl)-boronic acid in Example 1.

[0128] Tris[2,5-bis(dibenzofuran)-4-yl]pyridine-C³,N]iridium (III).

25 Example 31 (Synthesis of Ex. Comp. No. 150)

30 [0129] It is easy to synthesize the following compound in the same manner as in Example 2 except for using dibenzothiophene-4-boronic acid (made by Frontier Scientific Inc.) instead of 2-(9,9-dimethylfluorenyl)-boronic acid in Example 2.

[0130] Tris[2,5-bis(benzothiophene)-4-yl]pyridine-C³,N]iridium (III).

Example 32

35 [0131] An organic EL device shown in Figure 1C was prepared in the following manner.

[0132] On a 100 nm-thick patterned ITO electrode (anode) formed on a 1.1 mm-thick no-alkali glass substrate, a 40 nm-thick charge transport layer of α -NPD was formed by vacuum deposition (10^{-4} Pa) at a deposition rate of 0.1 nm/sec. On the charge transport layer, a 40 nm-thick luminescence layer (co-deposited film) of CBP: iridium complex of Ex. Comp. No. 23 (93:7 by weight) was formed by co-vacuum deposition at deposition rates of 0.1 nm/sec (for CBP) and 0.09 nm/sec (for the iridium complex) by controlling heating conditions of deposition vessel. On the luminescence layer, a 40 nm-thick exciton diffusion prevention layer of BCP (Bathocuproine) was formed by vacuum deposition at a deposition rate of 0.1 nm/sec, and/or the exciton diffusion prevention layer, a 20 nm-thick electron transport layer of Alq₃ was formed by vacuum deposition at a deposition rate of 0.1 nm/sec. Thereafter, or the electron transport layer, a 150 nm-thick aluminum electrode (cathode) was formed by vacuum deposition at a deposition rate of 1 nm/sec.

40 [0133] The thus-prepared organic EL device exhibited an EL spectrum showing $\lambda_{max} = 545$ nm and luminescent efficiencies of 12.4 1m/W at a luminance of 100 cd/m² and 13.6 1m/W at a luminance of 600 cd/m².

Example 33

45 [0134] An organic EL device was prepared and evaluated in the same manner as in Example 32 except for using Tris[2,5-bis(9,9-dimethylfluorene-2-yl)-pyridine-C³,N]iridium (III) (Ex. Comp. No. 43) in place of Tris[2-(9,9-dimethylfluorene-2-yl)pyridine-C³,N]iridium (III) (Ex. Comp. No. 23) synthesized in Example 1.

[0135] The thus-prepared organic EL device exhibited an EL spectrum showing $\lambda_{max} = 590$ nm and luminescent efficiencies of 2.4 1m/W at a luminance of 100 cd/m² and 1.9 1m/W at a luminance of 300 cd/m².

50 Example 34 (Synthesis of Ex. Comp. No. 54)

[0136] It is easy to synthesize the following compound in the same manner as in Example 1 except for using 4-phenyl-

1-bromopyridine (made by General Intermediates of Canada) instead of 2-bromopyridine in Example 1.
 [0137] Tris[2-(9,9-dimethylfluorene-2-yl)-4-phenylpyridine-C³,N]iridium (III).

[0138] As described above, according to the present invention, the metal coordination compound of the formula (1) characterized by the aromatic group of the formula (5) as a partial structure is an excellent material which exhibits a high emission quantum efficiency. The electroluminescence device (luminescence device) of the present invention using, as a luminescent center material, the metal coordination compound of the formula (1) is an excellent device which not only allows high-efficiency luminescence but also retains a high luminance for a long period and shows little deterioration by current passage. Further, the display apparatus using the electroluminescence device of the present invention exhibits excellent display performances.

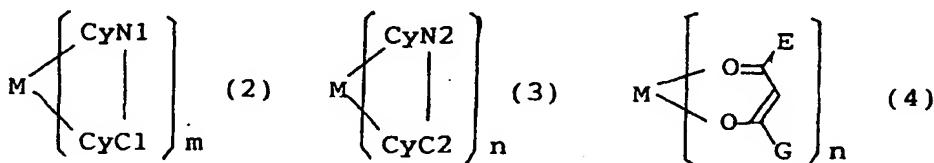
[0139] An electroluminescence device having a layer containing a specific metal coordination compound is provided. The metal coordination compound is represented by formula (1) below:



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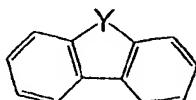
wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure MLm is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3) or (4) shown below:

20



25 at least one of the optional substituent(s) of the cyclic groups, and the cyclic groups CyC1 and CyC2 include an aromatic group capable of having a substituent represented by the following formula (5):

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40

[0140] The metal coordination compound having the aromatic group is effective in providing high-efficiency luminescence and long-term high luminance.

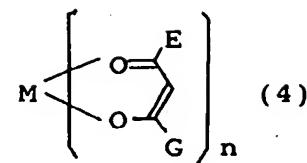
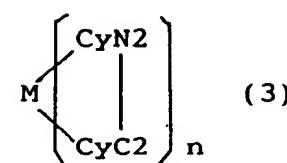
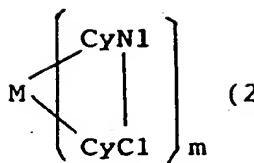
Claims

45 1. A metal coordination compound represented by formula (1) below:



50 wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure MLm is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3) or (4) shown below:

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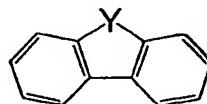


wherein CyN1 and CyN2 are each cyclic group capable of having a substituent, including a nitrogen atom and bonded to the metal atom M via the nitrogen atom; CyC1 and CyC2 are each cyclic group capable of having a substituent, including a carbon atom and bonded to the metal atom M via the carbon atom with the proviso that the cyclic group CyN1 and the cyclic group CyC1 are bonded to each other via a covalent bond and the cyclic group CyN2 and the cyclic group CyC2 are bonded to each other via covalent bond;

the optional substituent of the cyclic groups is selected from a halogen atom, cyano group, a nitro group, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom; a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom);

E and G are independently a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom; and

30 at least one of the optional substituent(s) of the cyclic groups, and the cyclic groups CyC1 and CyC2 include an aromatic group capable of having a substituent represented by the following formula (5):



(5)

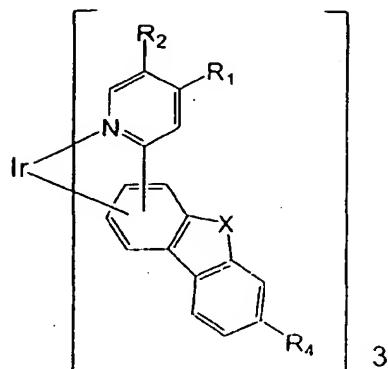
40 wherein the aromatic group of the formula (5) is bonded to CyN1, CyN2, CyC1 or CyC2 via a single bond when the aromatic group is the optional substituent(s) of the cyclic groups, and the aromatic group of the formula (5) is bonded to CyN1 or CyN2 via a single bond and bonded to the metal atom M via a single bond when the aromatic group is CyC1 or CyC2;

45 Y denotes C=O, CRR', C=C(CN)₂, O or S wherein R and R' are independently a hydrogen atom, a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a cyano atom, a nitro atom, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom); and

50 the optional substituent of the aromatic group of the formula (5) is selected from a halogen atom, cyano group, a nitro group, a trialkylsilyl group of which the alkyl groups are independently a linear or branched alkyl group having 1 to 8 carbon atoms, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom, or an aromatic group capable of having a substituent (that is a halogen atom, a

cyano atom, a nitro atom, a linear or branched alkyl group having 1 to 20 carbon atoms of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH- or -C≡C-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom) with the proviso that an adjacent pair of substituents can be bonded to form a cyclic structure.

- 5 2. A metal coordination compound according to Claim 1, including a partial structure ML'_n represented by the formula (3) in the formula (1).
- 10 3. A metal coordination compound according to Claim 1, including a partial structure ML'_n represented by the formula (4) in the formula (1).
- 15 4. A metal coordination compound according to Claim 1, wherein n is 0 in the formula (1).
- 15 5. A metal coordination compound according to Claim 1, wherein the group Y in the formula (5) is C=O or CRR'.
- 20 6. A metal coordination compound according to Claim 1, wherein the cyclic groups CyC1 and CyC2 are independently selected from phenyl group, thienyl group, thianaphthyl group, naphthyl group, pyrenyl group, 9-fluorenonyl group, fluorenyl group, dibenzofuryl group, dibenzothienyl group, or carbazolyl group, as an aromatic cyclic group capable of having a substituent with the proviso that the aromatic cyclic group can include one or two CH groups that can be replaced with a nitrogen atom.
- 25 7. A metal coordination compound according to Claim 6, wherein the cyclic groups CyC1 and Cy2 are independently phenyl group or 2-fluorenyl group.
- 25 8. A metal coordination compound according to Claim 1, wherein the cyclic groups CyN1 and CyN2 are independently selected from pyridyl group, pyridazinyl group, and pyrimidinyl group, as an aromatic cyclic group capable of having a substituent.
- 30 9. A metal coordination compound according to Claim 8, wherein the aromatic cyclic group is pyridyl group.
- 30 10. A metal coordination compound according to Claim 1, wherein the cyclic groups CyN1, CyN2, CyC1 and CyC2 are independently non-substituted, or have a substituent selected from a halogen atom and a linear or branched alkyl group having 1 to 20 carbon atoms {of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, -S-, -CO-, -CO-O-, -O-CO-, -CH=CH-, -C≡C-, or a divalent aromatic group capable of having a substituent (that is a halogen atom or a linear or branched alkyl group having 1 to 20 carbon atoms (of which the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O-, and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom)), and the alkyl group can include a hydrogen atom that can be optionally replaced with a fluorine atom}.
- 40 11. A metal coordination compound according to Claim 1, wherein M in the formula (1) is iridium.
- 45 12. A metal coordination compound according to Claim 1, which is represented by the following formula (6):



wherein X denotes CRR' , O or S where R and R' are independently a linear or branched alkyl group of formula: C_nH_{2n+1} in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom;

R2 denotes a hydrogen atom; a fluorine atom; a linear or branched alkyl group of formula: C_nH_{2n+1} in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom; a phenyl group capable of having a substituent; a 9,9-dialkylfluorenyl group (of which the alkyl groups are independently a linear or branched alkyl group of formula: C_nH_{2n+1} in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom); a dibenzofuranyl group capable of having a substituent; and a dibenzothienyl group capable of having a substituent; the optional substituent of phenyl group, 9,9-dialkylfluorenyl group, dibenzofuranyl group and dibenzothienyl group is a fluorine atom or a linear or branched alkyl group of formula: C_nH_{2n+1} in which n is an integer of 1 - 20, the alkyl group can include one or non-neighboring two or more methylene groups that can be replaced with -O- and also can include a hydrogen atom that can be optionally replaced with a fluorine atom.

35 13. An electroluminescence device, comprising: a pair of electrodes disposed on a substrate, and a luminescence unit comprising at least one organic compound disposed between the electrodes, wherein the organic compound comprises a metal coordination compound represented by the formula (1) in Claim 1.

40 14. An electroluminescence device according to Claim 13, wherein a voltage is applied between the electrodes to emit light.

15. An electroluminescence device according to Claim 13, wherein a voltage is applied between the electrodes to emit phosphorescence.

45 16. A picture display apparatus, comprising an electroluminescence device according to Claim 13, and a means for supplying electric signals to the electroluminescence device.

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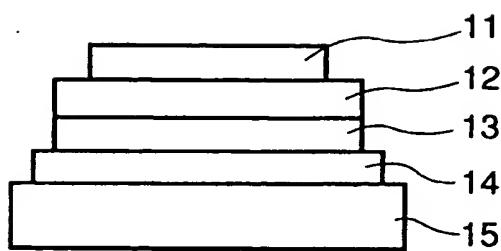


FIG. 1A

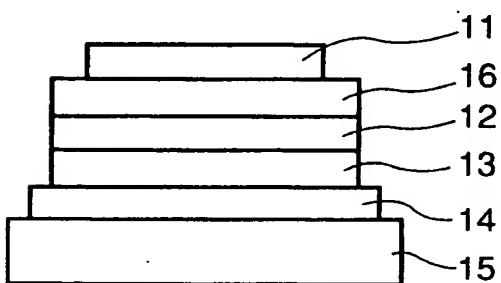


FIG. 1B

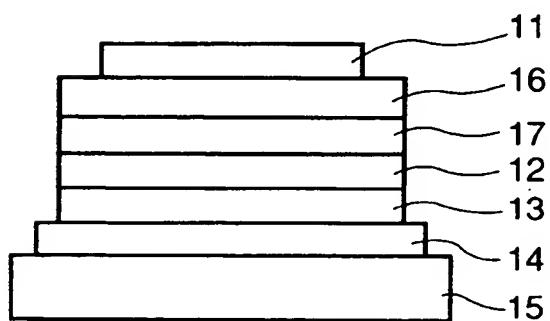


FIG. 1C

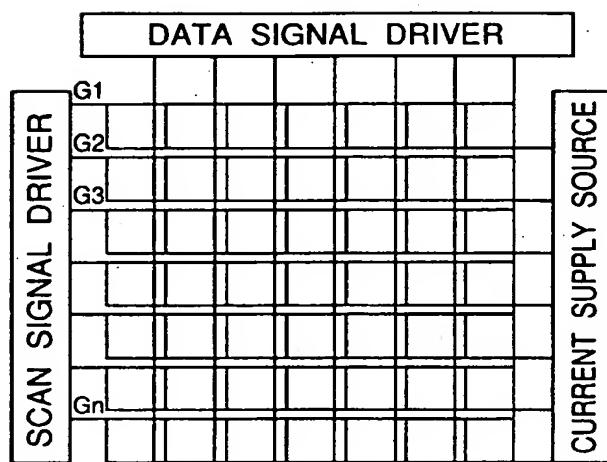


FIG. 2



(19)

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(11) EP 1 238 981 A3

(12)

EUROPEAN PATENT APPLICATION

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(51) Int Cl.7: C07F 15/00, H01L 51/00

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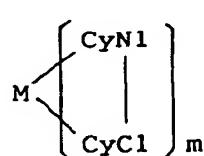
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(54) Metal coordination compound, luminescence device and display apparatus

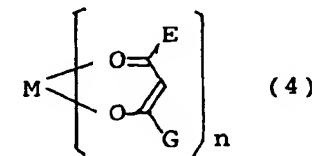
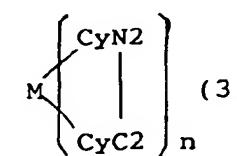
(57) An electroluminescence device having a layer containing a specific metal coordination compound is provided. The metal coordination compound is represented by formula (1) below:



wherein M is a metal atom of Ir, Pt, Rh or Pd; L and L' are mutually different bidentate ligands; m is 1, 2 or 3 and n is 0, 1 or 2 with the proviso that m+n is 2 or 3; a partial structure ML_m is represented by formula (2) shown below and a partial structure ML'_n is represented by formula (3) or (4) shown below:



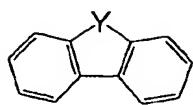
(2)



(4)

at least one of the optional substituent(s) of the cyclic groups, and the cyclic groups CyC1 and CyC2 include an aromatic group capable of having a substituent represented by the following formula (5):

EP 1 238 981 A3



The metal coordination compound having the aromatic group is effective in providing high-efficiency luminescence and long-term high luminance.



European Patent
Office

EUROPEAN SEARCH REPORT

Application Number
EP 02 00 5112

DOCUMENTS CONSIDERED TO BE RELEVANT			CLASSIFICATION OF THE APPLICATION (Int.Cl.)
Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	
X	BALDO M A ET AL: "VERY HIGH-EFFICIENCY GREEN ORGANIC LIGHT-EMITTING DEVICES BASED ON ELECTROPHOSPHORESCENCE" APPLIED PHYSICS LETTERS, AMERICAN INSTITUTE OF PHYSICS, NEW YORK, US, vol. 75, no. 1, 5 July 1999 (1999-07-05), pages 4-6, XP002949187 ISSN: 0003-6951 * the whole document * ---	1,4, 6-11, 13-16	C07F15/00 H01L51/00
X	DATABASE CA [Online] CHEMICAL ABSTRACTS SERVICE, COLUMBUS, OHIO, US; DJUROVICH, PETER I. ET AL: "Ir(III) cyclometalated complexes as efficient phosphorescent emitters in polymer blend and organic LEDs" retrieved from STN Database accession no. 132:300666 XP002200768 * abstract * & POLYMER PREPRINTS (AMERICAN CHEMICAL SOCIETY, DIVISION OF POLYMER CHEMISTRY) (2000); 41(1), 770-771.	1,4, 6-11, 13-16	
X	SERGEY LAMANSKY: "Molecularly doped polymer light emitting diodes utilizing phosphorescent Pt(II) and Ir(III) dopants" ORGANIC ELECTRONICS, ELSEVIER, AMSTERDAM, NL, no. 2, 2001, pages 53-62, XP002196402 ISSN: 1566-1199 page 55: Pt(thpy)2; FIr(ppy)3 * the whole document * ---	1,4, 6-11, 13-16	
The present search report has been drawn up for all claims			
Place of search	Date of completion of the search	Examiner	
MUNICH	31 May 2002	Richter, H	
CATEGORY OF CITED DOCUMENTS			
X : particularly relevant if taken alone Y : particularly relevant if combined with another document of the same category A : technological background O : non-written disclosure P : intermediate document			
T : theory or principle underlying the invention E : earlier patent document, but published on, or after the filing date D : document cited in the application L : document cited for other reasons & : member of the same patent family, corresponding document			



European Patent
Office

Application Number
EP 02 00 5112

CLAIMS INCURRING FEES

The present European patent application comprised at the time of filing more than ten claims.

- Only part of the claims have been paid within the prescribed time limit. The present European search report has been drawn up for the first ten claims and for those claims for which claims fees have been paid, namely claim(s):

- No claims fees have been paid within the prescribed time limit. The present European search report has been drawn up for the first ten claims.

LACK OF UNITY OF INVENTION

The Search Division considers that the present European patent application does not comply with the requirements of unity of Invention and relates to several inventions or groups of inventions, namely:

see sheet B

- All further search fees have been paid within the fixed time limit. The present European search report has been drawn up for all claims.

- As all searchable claims could be searched without effort justifying an additional fee, the Search Division did not invite payment of any additional fee.

- Only part of the further search fees have been paid within the fixed time limit. The present European search report has been drawn up for those parts of the European patent application which relate to the inventions in respect of which search fees have been paid, namely claims:

- None of the further search fees have been paid within the fixed time limit. The present European search report has been drawn up for those parts of the European patent application which relate to the invention first mentioned in the claims, namely claims:

4, 12, partially: 1,5 - 11, 13 - 16

European Patent
Office

EUROPEAN SEARCH REPORT

Application Number

EP 02 00 5112

DOCUMENTS CONSIDERED TO BE RELEVANT									
Category	Citation of document with indication, where appropriate, of relevant passages	Relevant to claim	CLASSIFICATION OF THE APPLICATION (Int.Cl.)						
P,X	WO 02 02714 A (E.I. DU PONT DE NEMOURS AND COMPANY, USA) 10 January 2002 (2002-01-10) fourth formula : fac-Ir(La)3 fifth formula mer-Ir(La)3 * page 6, line 1 - page 10, line 19; claims 1-8; example 1; tables 2-4 * ---	1,4, 6-11, 13-16							
P,X	WO 02 15645 A (THE TRUSTEES OF PRINCETON UNIVERSITY, USA; THE UNIVERSITY OF SOUTHERN C) 21 February 2002 (2002-02-21) * claims 3,5,9,29; figures 7P,8C *	1,4, 6-11, 13-16							
E	EP 1 191 612 A (CANON KABUSHIKI KAISHA, JAPAN) 27 March 2002 (2002-03-27) * the whole document *	1,4, 6-11, 13-16							
E	EP 1 191 613 A (CANON KABUSHIKI KAISHA, JAPAN) 27 March 2002 (2002-03-27) * the whole document *	1,4, 6-10, 13-16	TECHNICAL FIELDS SEARCHED (Int.Cl.)						
E	EP 1 191 614 A (CANON KABUSHIKI KAISHA, JAPAN) 27 March 2002 (2002-03-27) * page 5 - page 23; examples 2,4-8,11-13,16,18-20,23; table 8 *	1,4, 6-10, 13-16							
<p>The present search report has been drawn up for all claims</p> <table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <td style="width: 33%;">Place of search</td> <td style="width: 33%;">Date of completion of the search</td> <td style="width: 33%;">Examiner</td> </tr> <tr> <td>MUNICH</td> <td>31 May 2002</td> <td>Richter, H</td> </tr> </table> <p>CATEGORY OF CITED DOCUMENTS</p> <p>X : particularly relevant if taken alone Y : particularly relevant if combined with another document of the same category A : technological background O : non-written disclosure P : intermediate document</p> <p>T : theory or principle underlying the invention E : earlier patent document, but published on, or after the filing date D : document cited in the application L : document cited for other reasons & : member of the same patent family, corresponding document</p>				Place of search	Date of completion of the search	Examiner	MUNICH	31 May 2002	Richter, H
Place of search	Date of completion of the search	Examiner							
MUNICH	31 May 2002	Richter, H							



European Patent
Office

LACK OF UNITY OF INVENTION
SHEET B

Application Number
EP 02 00 5112

The Search Division considers that the present European patent application does not comply with the requirements of unity of invention and relates to several inventions or groups of inventions, namely:

1. Claims: 4, 12; partially: 1,5-11,13-16
complexes of formula (I) in which n is 0
2. Claims: 2, partially: 1, 5-11,13-16
complexes of formula (I) in which n is not 0 and the partial structure ML'n is represented by formula (3)
3. Claims: 3; partially: 1, 5-11,13-16
complexes of formula (I) in which n is not 0 and the partial structure ML'n is represented by formula (4)

ANNEX TO THE EUROPEAN SEARCH REPORT
ON EUROPEAN PATENT APPLICATION NO.

EP 02 00 5112

This annex lists the patent family members relating to the patent documents cited in the above-mentioned European search report.
 The members are as contained in the European Patent Office EDP file on
 The European Patent Office is in no way liable for these particulars which are merely given for the purpose of information.

31-05-2002

Patent document cited in search report		Publication date		Patent family member(s)		Publication date
WO 0202714	A	10-01-2002	AU WO	7155001 A 0202714 A2	14-01-2002 10-01-2002	
WO 0215645	A	21-02-2002	AU WO	8327401 A 0215645 A1	25-02-2002 21-02-2002	
EP 1191612	A	27-03-2002	EP US	1191612 A2 2002063516 A1	27-03-2002 30-05-2002	
EP 1191613	A	27-03-2002	EP US	1191613 A2 2002064681 A1	27-03-2002 30-05-2002	
EP 1191614	A	27-03-2002	JP EP US	2002175884 A 1191614 A2 2002068190 A1	21-06-2002 27-03-2002 06-06-2002	